

Simplifying Quantum Circuits via Circuit Invariants and Dressed CNOTs

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Abstract

Quantum Compiling Algorithms decompose (exactly, without approximations) an arbitrary 2^{N_B} unitary matrix acting on N_B qubits, into a sequence of elementary operations (SEO). There are many possible ways of decomposing a unitary matrix into a SEO, and some of these decompositions have shorter length (are more efficient) than others. Finding an optimum (shortest) decomposition is a very hard task, and is not our intention here. A less ambitious, more doable task is to find methods for optimizing small segments of a SEO. Call these methods piecewise optimizations. Piecewise optimizations involve replacing a small quantum circuit by an equivalent one with fewer CNOTs. Two circuits are said to be equivalent if one of them multiplied by some external local operations equals the other. This equivalence relation between circuits has its own class functions, which we call circuit invariants. Dressed CNOTs are a simple yet very useful generalization of standard CNOTs. After discussing circuit invariants and dressed CNOTs, we give some methods for simplifying 2-qubit and 3-qubit circuits. We include with this paper software (written in Octave/Matlab) that checks many of the algorithms proposed in the paper.

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1 Introduction

Quantum Compiling Algorithms decompose (exactly, without approximations) an arbitrary 2^{N_B} unitary matrix acting on N_B qubits, into a sequence of elementary operations (SEO). By elementary operations we mean operations that act on only a few

(usually 1 or 2) qubits (for example, all single-qubit rotations and CNOTs.) The most efficient quantum compiling algorithms to date are based on a recursive application of the Cosine-Sine Decomposition (CSD), a technique first proposed in Ref.[1]. An implementation of the algorithm of Ref.[1] may be found in the computer program called Qubiter (patented, C++ source code publicly available at www.ar-tiste.com). Long after Ref.[1] and Qubiter came out, many papers on quantum compiling via recursive CSD have appeared. These can be easily tracked down by making a keyword search in ArXiv or Google for something like (“Cosine-Sine” and “Decomposition” and “quantum”) .

We will call the number of CNOTs in a SEO its length. (Single-qubit rotations are not counted because these can be performed much faster than CNOTs.) Of course, there are many possible ways of decomposing a unitary matrix into a SEO, and some of these decompositions have shorter length (are more efficient) than others. The algorithm of Ref.[1] per se does not yield the shortest SEO. Finding an optimum (shortest) decomposition is a very hard task, and is not our intention here. A less ambitious, more doable task is to find methods for optimizing small segments of a SEO. Call these methods piecewise optimizations. The hope is that given any SEO, one can apply piecewise optimization methods to reduce the original SEO into an equivalent SEO whose length is much less, and might even be close to the shortest possible length. An analogy to our piecewise optimization strategy is the following. Think of a SEO as being like a path between two points in a manifold. If this path is initially unnecessary long, one might hope to make it a little less so by breaking it into pieces and optimizing the length of each piece. Breaking it into pieces again, and optimizing each piece again. And so on.

Piecewise optimizations involve replacing a small quantum circuit by an equivalent one with fewer CNOTs. Two circuits are said to be equivalent if one of them multiplied by some external local operations equals the other. By external local operations, we mean single-qubit rotations applied at the beginning or end of the circuit. This equivalence relation between circuits has its own class functions, which we call circuit invariants. Many excellent papers already exist on the use of such invariants in quantum computing. See, for example, Refs. [2], [3], [4], and [5]. Such invariants are a crucial ingredient of this paper. (However, the paper does not assume that the reader possesses any prior knowledge about these invariants. The paper is self-contained in this regard.)

Besides circuit invariants, another important ingredient of this paper is what we call dressed CNOTs (DC-NOTs). DC-NOTs are a simple yet very useful generalization of standard CNOTs. To my knowledge, this paper is the first one to consider DC-CNOTs. DC-NOTs are convenient because they lump together a CNOT and some single-qubit rotations. Modulo external local operations, one can express any circuit solely in terms of a single type of circuit element (DC-CNOTs), rather than having to express it with two different types of circuit elements (CNOTs and single-qubit rotations).

After discussing circuit invariants and DC-NOTs, this paper gives some methods for simplifying 2-qubit and 3-qubit circuits.

Much is already known about simplifying 2-qubit circuits. Ref.[6] shows, via Cartan’s KAK decomposition[7], that a 2-qubit circuit with any number of CNOTs can always be reduced to a circuit with 3 CNOTs. Refs.[6] and [5] give necessary and sufficient conditions for when a 2-qubit circuit with 3 CNOTs reduces to fewer than 3 CNOTs. In this paper, we spend some time re-proving these already known 2-qubit results using the new language of circuit invariants and DC-NOTs. This exercise yields new techniques and new geometrical insights that were lacking in previous proofs.

In this paper, we also present some interesting new ways of simplifying 3-qubit circuits. Our results for 3-qubit circuits rely heavily on our results for 2-qubit circuits.

We include with this paper software (written in Octave/Matlab) that checks many of the algorithms proposed in the paper. In the header of each section, and in the Table of Contents, each section name is followed by a list in square brackets of the names of the Octave m-files relevant to that section. Our software is not intended to be very efficient, or to be free of all conceivable loopholes. It is only intended to be a proof of principle of our algorithms.

2 Notation

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[ global_declarations.m, global_defs.m, simul_real_svd.m, Gamma_rep.m,
sig.m, check_dcnots.m, factor_SU2pow2_matrix.m, factor_SU2pow3_matrix.m,
test_factor_su2pow.m, get_normal_unit_vec.m, get_unit_vec.m ]
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In this section, we discuss notation, linguistic idiosyncrasies and abbreviations that will be used in subsequent sections. If any notation in this paper remains unclear to the reader after reading this section, he should consult Ref.[8], a review article, written by the author of this paper, that uses the same notation as this paper.

We will often use the symbol $N_B = 0, 1, 2, \dots$ for number of bits, and $N_S = 2^{N_B}$ for the corresponding number of states.

We will often abbreviate $\cos(\alpha)$ and $\sin(\alpha)$ by c_α and s_α , respectively. We will often use a subscript of f to denote the final value of quantity that changes (e.g., \hat{a} changes to \hat{a}_f). When we say $b = \pm a$, we mean $b \in \{a, -a\}$. When we write $X_{\alpha \rightarrow \beta}$, we mean, the quantity obtained by replacing α by β everywhere in X . Likewise, by $X_{\alpha \leftrightarrow \beta}$ we mean, the quantity obtained by swapping α and β everywhere in X . When we say “ $A(\textit{ditto}, A')$ is $B(\textit{ditto}, B')$ ” we mean “ A is B and A' is B' ”. LHS and RHS will stand for left-hand side and right-hand side. “RHON basis” will stand for “right-handed orthonormal basis”.

Let $Bool = \{0, 1\}$. Let \mathbb{R} denote the real numbers, \mathbb{C} the complex numbers, \mathbb{Z} all integers (positive and negative). For integers a and b , $\mathbb{Z}_{a,b}$ will denote all integers

from a to b , including a and b . If Ω is anyone of the symbols $>, \geq, <, \leq$, and S is any set, define $S^{\Omega 0} = \{x \in S : x \Omega 0\}$ if the right hand side is defined. For example, $\mathbb{Z}^{>0}$ are the positive integers. As usual, for any set S and $r, p, q \in \mathbb{Z}^{>0}$, S^r will denote the set of r -tuples of S , and $S^{p \times q}$, the set of $p \times q$ matrices with entries in S .

As usual, $U(N_S)$ will denote the $N_S \times N_S$ unitary matrices, and $SU(N_S)$ the special (i.e., with determinant=1) elements of $U(N_S)$. Given any $A \in U(N_S)$, we define \hat{A} by $\hat{A} = A/[\det(A)]^{\frac{1}{N_S}}$, where we choose the principal branch of the function $(\cdot)^{\frac{1}{N_S}}$. We will refer to \hat{A} as the “special counterpart” of A . (here the adjective “special” again means “with determinant=1”).

\mathbb{R}^3 will denote the set of all 3 dimensional real vectors, and $\mathbb{R}^3 = \{x \in \mathbb{R}^3 : |x| = 1\}$. As is common in the Physics literature, a letter with an arrow (ditto, caret) over it, as in \vec{a} (ditto, \hat{a}) will denote an element of \mathbb{R}^3 (ditto, \mathbb{R}^3). \vec{a} and \hat{a} will be treated as column vectors when they appear in matrix expressions.

Let $\vec{a}_j \in \mathbb{R}^3$ for $j \in \mathbb{Z}_{1,r}$. We will use the following non-standard notation for r -fold cross products:

$$[\vec{a}_1 \vec{a}_2 \vec{a}_3 \dots \vec{a}_r] = (\dots ((\vec{a}_1 \times \vec{a}_2) \times \vec{a}_3) \dots \times \vec{a}_r) . \quad (1)$$

For example, $[\vec{a}_1 \vec{a}_2 \vec{a}_3 \vec{a}_4] = ((\vec{a}_1 \times \vec{a}_2) \times \vec{a}_3) \times \vec{a}_4$. Of course, an $(r+2)$ -fold cross-product can be reduced to an r -fold cross-product using the well known “BAC minus CAB” identities: for $\vec{a}, \vec{b}, \vec{c} \in \mathbb{R}^3$, $\vec{a} \times (\vec{b} \times \vec{c}) = \vec{b}(\vec{a} \cdot \vec{c}) - \vec{c}(\vec{a} \cdot \vec{b})$ and $(\vec{a} \times \vec{b}) \times \vec{c} = \vec{b}(\vec{a} \cdot \vec{c}) - \vec{a}(\vec{b} \cdot \vec{c})$. For example, if \hat{a}, \hat{b} are perpendicular unit vectors, then $[\hat{a} \hat{b} \hat{b}] = -\hat{a}$.

Suppose $\vec{a}, \vec{b} \in \mathbb{R}^3$. $\text{angle}(\vec{a}, \vec{b})$ will denote the angle between \vec{a} and \vec{b} , defined up to 2π . We will say \vec{a} is parallel to \vec{b} and write $\vec{a} \parallel \vec{b}$ iff $\vec{a} \times \vec{b} = 0$; i.e., iff $\vec{a} = \pm \vec{b}$, or $\vec{a} = 0$, or $\vec{b} = 0$. We will say \vec{a} is perpendicular to \vec{b} and write $\vec{a} \perp \vec{b}$ iff $\vec{a} \cdot \vec{b} = 0$. For $\vec{b} \neq 0$, define $\vec{a}_{\parallel \vec{b}}$, **the part of \vec{a} along \vec{b}** , by

$$\vec{a}_{\parallel \vec{b}} = \frac{(\vec{a} \cdot \vec{b})\vec{b}}{|\vec{b}|^2} . \quad (2)$$

For $\vec{b} \neq 0$, define $\vec{a}_{\perp \vec{b}}$, **the part of \vec{a} across \vec{b}** , by

$$\vec{a}_{\perp \vec{b}} = \vec{a} - \vec{a}_{\parallel \vec{b}} = \vec{a} - \frac{(\vec{a} \cdot \vec{b})\vec{b}}{|\vec{b}|^2} = \frac{-[\vec{a} \vec{b} \vec{b}]}{|\vec{b}|^2} . \quad (3)$$

For any square matrix A , A^T will denote its transpose, A^* , its complex conjugate, and $A^\dagger = A^{*T}$, its Hermitian conjugate. $\delta_{i,j}$ will denote the Kronecker delta function. (It equals one if $i = j$ and zero otherwise.)

Let $I_2, \sigma_X, \sigma_Y, \sigma_Z$ be the 2d identity matrix and Pauli matrices. Sometimes, we set $(X_1, X_2, X_3) = (X, Y, Z)$ and denote the Pauli matrices by $\sigma_{X_1}, \sigma_{X_2}, \sigma_{X_3}$. Suppose $W \in \{X, Y, Z\}$. Define the number operators: $n_W = \frac{1-\sigma_W}{2}$ and $\bar{n}_W = \frac{1+\sigma_W}{2}$. Note that $(-1)^{n_W} = \sigma_W$. Usually, n_Z is denoted merely by n and \bar{n}_Z by \bar{n} . If $W_j \in$

$\{1, X, Y, Z\}$ for $j \in \mathbb{Z}_{1, N_B}$, let $\sigma_{W_1, W_2, \dots, W_{N_B}} = \sigma_{W_1} \otimes \sigma_{W_2} \otimes \dots \otimes \sigma_{W_{N_B}}$, where any incidence of σ_1 on the RHS is replaced by I_2 . For example, $\sigma_{XY1} = \sigma_X \otimes \sigma_Y \otimes I_2$.

$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ is the one-bit Hadamard matrix and $H^{\otimes N_B}$ is its N_B -fold tensor product. H satisfies $H^2 = 1$, $H\sigma_X H = \sigma_Z$, $H\sigma_Z H = \sigma_X$ and $H\sigma_Y H = -\sigma_Y$.

Suppose $a_0 \in \mathbb{R}$ and $\vec{a} \in \mathbb{R}^3$. We will abbreviate $\vec{\sigma} \cdot \vec{a}$ by $\sigma_{\vec{a}}$. The standard terminology is to call $a_0 + i\sigma_{\vec{a}}$ a **quaternion**, and to call $\sigma_{\vec{a}}$ a vector quaternion (divided by i). To shorten this terminology, we will refer to $\sigma_{\vec{a}}$ as a **Paulion**, and call \vec{a} its **defining vector**. If $|\vec{a}| = 1$, we will call $\sigma_{\vec{a}}$ a **unit Paulion**. One can reduce a product of two Paulions by using the identity $\sigma_{\vec{a}}\sigma_{\vec{b}} = \vec{a} \cdot \vec{b} + i\sigma_{\vec{a} \times \vec{b}}$. For $\hat{a} \in \hat{\mathbb{R}}^3$, define number operators $n_{\hat{a}} = \frac{1-\sigma_{\hat{a}}}{2}$ and $\bar{n}_{\hat{a}} = \frac{1+\sigma_{\hat{a}}}{2}$. Note that $(-1)^{n_{\hat{a}}} = \sigma_{\hat{a}}$. If $W_j \in \hat{\mathbb{R}}^3$ or $W_j = 1$ for $j \in \mathbb{Z}_{1, N_B}$, let $\sigma_{W_1, W_2, \dots, W_{N_B}} = \sigma_{W_1} \otimes \sigma_{W_2} \otimes \dots \otimes \sigma_{W_{N_B}}$.

Suppose \mathcal{M} is the set of all matrices $M \in \mathbb{C}^{4 \times 4}$ that can be expressed in the form $M = \sum_k \sigma_{\vec{a}_k, \vec{b}_k}$, where $\vec{a}_k, \vec{b}_k \in \mathbb{R}^3$ for all k . Suppose \mathcal{L} is the set of all matrices $L \in \mathbb{R}^{3 \times 3}$ that can be expressed in the form $L = \sum_k \vec{a}_k \vec{b}_k^T$, where $\vec{a}_k, \vec{b}_k \in \mathbb{R}^3$ for all k . For every $M \in \mathcal{M}$, let $\Gamma(M)$ or M^Γ represent the 3×3 matrix with entries $\frac{1}{4}\text{tr}(\sigma_{X_i, X_j} M)$, where $i, j \in \mathbb{Z}_{1, 3}$. (The symbol Γ was chosen to evoke the mental picture of a column vector times a row vector; such is the output of the function $\Gamma(\cdot)$). For every $L \in \mathcal{L}$, define $\Gamma^{-1}(L) = \sum_{i, j} \sigma_{X_i, X_j} L_{i, j}$. It's easy to check that $\Gamma\Gamma^{-1} = \Gamma^{-1}\Gamma = 1$ so the map $\Gamma : \mathcal{M} \rightarrow \mathcal{L}$ is 1-1 onto. Let $\text{lin}(\mathcal{M})$ be the set of linear combinations over \mathbb{C} of elements of \mathcal{M} , and $\text{lin}(\mathcal{L})$ of \mathcal{L} . The map Γ can be extended to $\bar{\Gamma} : \mathbb{C} + \text{lin}(\mathcal{M}) \rightarrow \mathbb{C} + \text{lin}(\mathcal{L})$, $\bar{\Gamma}(\lambda + \sum_i \alpha_i M_i) = \lambda + \sum_i \alpha_i M_i^\Gamma$. $\bar{\Gamma}$ is also a 1-1 onto map. Henceforth, we will use Γ to refer to both Γ and its extension $\bar{\Gamma}$. Given a matrix $A \in \mathbb{C} + \text{lin}(\mathcal{M})$, we will call A^Γ its Gamma representation. Often, in contexts where this will not lead to confusion, we will drop the Γ superscript and denote A^Γ simply by A .

The next theorem, although almost trivial, will be used frequently in this paper.

Theorem 1 *The map $f : \hat{\mathbb{R}}^3 \times \hat{\mathbb{R}}^3 \rightarrow SU(2)$, $f(\hat{a}, \hat{b}) = \sigma_{\hat{a}}\sigma_{\hat{b}}$ is well defined and onto. In other words: (well-defined) If $\hat{a}, \hat{b} \in \hat{\mathbb{R}}^3$, then $f(\hat{a}, \hat{b}) \in SU(2)$. (onto) If $U \in SU(2)$, then there exist $\hat{a}, \hat{b} \in \hat{\mathbb{R}}^3$ such that $U = f(\hat{a}, \hat{b})$.*

proof:

(well defined) Given $\hat{a}, \hat{b} \in \hat{\mathbb{R}}^3$, one can always find an angle θ such that $\hat{a} \cdot \hat{b} = c_\theta$ and $|\hat{a} \times \hat{b}| = s_\theta$. Let $\hat{w} = \frac{\hat{a} \times \hat{b}}{|\hat{a} \times \hat{b}|}$. It follows that $\sigma_{\hat{a}}\sigma_{\hat{b}} = \hat{a} \cdot \hat{b} + i\sigma_{\hat{a} \times \hat{b}} = e^{i\theta\sigma_{\hat{w}}} \in SU(2)$.

(onto) Given $U = e^{i\theta\sigma_{\hat{w}}}$, where $\hat{w} \in \hat{\mathbb{R}}^3$ and $\theta \in \mathbb{R}$, one can always find a (non-unique) pair of unit vectors \hat{a} and \hat{b} in the plane perpendicular to \hat{w} , such that $\theta = \text{angle}(\hat{a}, \hat{b})$, and $\hat{a} \times \hat{b}$ points in the \hat{w} direction. Hence, $\hat{a} \cdot \hat{b} = c_\theta$ and $\hat{a} \times \hat{b} = s_\theta \hat{w}$. It follows that $\sigma_{\hat{a}}\sigma_{\hat{b}} = \hat{a} \cdot \hat{b} + i\sigma_{\hat{a} \times \hat{b}} = e^{i\theta\sigma_{\hat{w}}}$.

QED

One has:

$$\sigma_{\hat{r}}\sigma_{\hat{a}}\sigma_{\hat{r}} = \sigma_{\hat{r}}(\sigma_{\hat{a}_{\parallel\hat{r}}} + \sigma_{\hat{a}_{\perp\hat{r}}})\sigma_{\hat{r}} = \sigma_{\hat{a}_{\parallel\hat{r}}} - \sigma_{\hat{a}_{\perp\hat{r}}} = \sigma_{\hat{a}_{\parallel\hat{r}} - \hat{a}_{\perp\hat{r}}} = \sigma_{\hat{a}_f} . \quad (4)$$

A geometrical interpretation of this identity is shown in Fig.1a. The similarity transformation $\sigma_{\hat{r}}(\cdot)\sigma_{\hat{r}}$ takes the Paulion $\sigma_{\hat{a}}$ to $\sigma_{\hat{a}_f}$, where \hat{a}_f is the reflection of \hat{a} on \hat{r} .

Suppose $\hat{a}, \hat{b} \in \mathbb{R}^3$, and we want to find $U \in SU(2)$ such that $\sigma_{\hat{b}} = U^\dagger \sigma_{\hat{a}} U$. Such a U can be constructed as a product of two Paulions (See Fig.1b). Indeed, let $\theta = \text{angle}(\hat{a}, \hat{b})$ and $\hat{p} = \frac{\hat{a} \times \hat{b}}{|\hat{a} \times \hat{b}|}$. Let \hat{r} be the vector that bisects the angle between \hat{a} and \hat{b} , and is oriented so that $\hat{a} \times \hat{r}$ points along \hat{p} . Note that \hat{b} can be obtained by reflecting \hat{a} on the bisector \hat{r} . Hence

$$\sigma_{\hat{a}}\sigma_{\hat{r}} = e^{i\frac{\theta}{2}\sigma_{\hat{p}}} , \quad \sigma_{\hat{b}} = \sigma_{\hat{r}}\sigma_{\hat{a}}\sigma_{\hat{r}} . \quad (5)$$

Combining these two results yields

$$\sigma_{\hat{b}} = (\sigma_{\hat{r}}\sigma_{\hat{a}})\sigma_{\hat{a}}(\sigma_{\hat{a}}\sigma_{\hat{r}}) = e^{-i\frac{\theta}{2}\sigma_{\hat{p}}}\sigma_{\hat{a}}e^{i\frac{\theta}{2}\sigma_{\hat{p}}} . \quad (6)$$

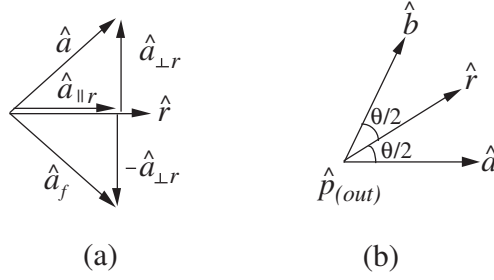


Figure 1: (a) If $\sigma_{\hat{r}}\sigma_{\hat{a}}\sigma_{\hat{r}} = \sigma_{\hat{a}_f}$, then \hat{a}_f is obtained by reflecting \hat{a} on \hat{r} . (b) Suppose \hat{b} is the result of rotating \hat{a} by an angle θ . Then \hat{b} can be obtained by reflecting \hat{a} on the bisector \hat{r} of the angle between \hat{a} and \hat{b} .

3 Invariants for Quantum Circuits

In this section, we will discuss circuit invariants; i.e., functions that map all equivalent circuits to the same value. By equivalent circuits we mean circuits that are equal, modulo external local operations.

Suppose A and B are elements of $U(N_S)$ (i.e., they are N_B -qubit gates). We will say A and B are **equivalent under local operations on the right hand side (LO-RHS)**, and write $A \sim_R B$, iff there exist $U_j \in U(2)$ for $j \in \mathbb{Z}_{0, N_B-1}$ such that

$$B = A(U_{N_B-1} \otimes \dots \otimes U_2 \otimes U_1 \otimes U_0) . \quad (7)$$

\sim_R is clearly an equivalence relation as it is symmetric, reflexive and transitive.

Henceforth, we will say that a function χ with domain $U(N_S)$ is a LO-RHS invariant if for any $A, B \in U(N_S)$, $A \sim_R B$ implies that $\chi(A) = e^{i\zeta} \chi(B)$ for some $\zeta \in \mathbb{R}$ (ζ may depend on A, B).

A frequent goal is to find a complete set of scalar invariant functions; that is, a set of functions $\chi_j : U(N_S) \rightarrow \mathbb{R}$ such that for any $A, B \in U(N_S)$, $A \sim_R B$ if and only if $\chi_j(A) = \chi_j(B)$ for all j . An extensive literature already exist on such invariants. They were first studied by Group Theorists, and, in more recent times, they have been used by Quantum Computerists [2], [3], [4], [5].

One can define an analogous equivalence relation \sim_L for local operations on the left hand side (LO-LHS), and an equivalence relation \sim_{LR} for local operations on both sides (LO-2S). Of course, the equivalence classes (e-classes) of \sim_R are a disjoint partition of $U(N_S)$. Ditto for the e-classes of \sim_L and \sim_{LR} . It's also clear that any e-class for \sim_R is contained in an e-class for \sim_{LR} , and that some e-classes of \sim_{LR} contain more than one e-class of \sim_R . (In fact, the e-classes of \sim_R contained within a single e-class of \sim_{LR} , can be labeled by the elements of $U(2)^{\otimes N_B}$).

Note that for any $\vec{a} \in \mathbb{R}^3$,

$$\sigma_Y \sigma_{\vec{a}}^T \sigma_Y = -\sigma_{\vec{a}}. \quad (8)$$

Hence, for $\theta \in \mathbb{R}$ and $\vec{a} \in \mathbb{R}^3$,

$$\sigma_Y [e^{i(\theta + \sigma_{\vec{a}})}]^T \sigma_Y = e^{i(\theta - \sigma_{\vec{a}})}. \quad (9)$$

Thus, when $U \in SU(2)$ (but not when $U \in U(2)$), $\sigma_Y U^T \sigma_Y = U^{-1} = U^\dagger$.

For any $A \in U(N_S)$, define a quadratic (second order in A) invariant

$$A^{(2)} = A \sigma_Y^{\otimes N_B} A^T \sigma_Y^{\otimes N_B}. \quad (10)$$

For example, for $A \in U(4)$, $A^{(2)} = A \sigma_{YY} A^T \sigma_{YY}$.

Theorem 2

(a) For $A, B \in SU(4)$, $A \sim_R B$ if and only if $A^{(2)} = (-1)^n B^{(2)}$ for some $n \in \mathbb{Z}$.

(b) For $A, B \in U(4)$, $A \sim_R B$ if and only if $A^{(2)} = e^{i\zeta} B^{(2)}$ for some $\zeta \in \mathbb{R}$.

proof:

(a) Assume $A, B \in SU(4)$. A can always be represented in the form

$$A = i^{n(A)} \exp(ia_{jk} \sigma_{X_j X_k}) \exp(ia'_j \sigma_{X_j 1}) \exp(ia_k \sigma_{1 X_k}), \quad (11)$$

where $n(A) \in \mathbb{Z}$ and $a_{jk}, a'_j, a_k \in \mathbb{R}$. (Note that $\det(iI_4) = 1$ so $\det(A) = 1$.) We are using Einstein's implicit summation convention, and j, k range over $\{1, 2, 3\}$. By Eqs.(8) and (11),

$$\sigma_{YY} A^T \sigma_{YY} = i^{n(A)} \exp(-ia_k \sigma_{1X_k}) \exp(-ia'_j \sigma_{X_j 1}) \exp(ia_{jk} \sigma_{X_j X_k}) . \quad (12)$$

Thus

$$A^{(2)} = (-1)^{n(A)} \exp(i2a_{jk} \sigma_{X_j X_k}) . \quad (13)$$

Likewise, B can be represented in the form

$$B = i^{n(B)} \exp(ib_{jk} \sigma_{X_j X_k}) \exp(ib'_j \sigma_{X_j 1}) \exp(ib_k \sigma_{1X_k}) , \quad (14)$$

where $n(B) \in \mathbb{Z}$ and $b_{jk}, b'_j, b_k \in \mathbb{R}$. Then

$$B^{(2)} = (-1)^{n(B)} \exp(i2b_{jk} \sigma_{X_j X_k}) . \quad (15)$$

(\Rightarrow) Suppose $A \sim_R B$. Looking at Eqs.(7), (11) and (14), we see that for every j, k , there exists an integer n_{jk} such that $a_{jk} = b_{jk} + \pi n_{jk}$. Therefore,

$$\exp(i2a_{jk} \sigma_{X_j X_k}) = \exp(i2b_{jk} \sigma_{X_j X_k}) . \quad (16)$$

Therefore, looking at Eqs.(13) and (15), we see that there exists an integer n such that $A^{(2)} = (-1)^n B^{(2)}$.

(\Leftarrow) Suppose $A^{(2)} = (-1)^n B^{(2)}$. Then, looking at Eqs.(13) and (15), we see that for every j, k , there exists an integer n_{jk} such that $2a_{jk} = 2b_{jk} + \pi n_{jk}$. Therefore,

$$\exp(ia_{jk} \sigma_{X_j X_k}) = \exp(ib_{jk} \sigma_{X_j X_k}) \prod_{j,k} [i \sigma_{X_j X_k}]^{n_{jk}} . \quad (17)$$

Therefore, from Eqs.(7), (11) and (14), we see that $A \sim_R B$.

- (b) Assume $A, B \in U(4)$. Eqs.(11) and (13) still apply except that we must replace in them $i^{n(A)}$ by $e^{i\zeta(A)}$ and $(-1)^{n(A)}$ by $e^{i2\zeta(A)}$ for some $\zeta(A) \in \mathbb{R}$. Eqs.(14) and (15) still apply except that we must replace in them $i^{n(B)}$ by $e^{i\zeta(B)}$ and $(-1)^{n(B)}$ by $e^{i2\zeta(B)}$ for some $\zeta(B) \in \mathbb{R}$.

(\Rightarrow) Suppose $A \sim_R B$. Eq.(16) still applies so there exists $\zeta \in \mathbb{R}$ such that $A^{(2)} = e^{i\zeta} B^{(2)}$.

(\Leftarrow) Suppose $A^{(2)} = e^{i\zeta} B^{(2)}$. Eq.(17) still applies so $A \sim_R B$.

QED

By virtue of Theorem 2, the absolute value of the entries of the matrix $A^{(2)}$ are a complete set of LO-RHS scalar invariants for $N_B = 2$. Theorem 2(a) reflects the fact that when $A, B \in SU(4)$, since A and B must both have unit determinant, the only local operations connecting A and B are either elements of $SU(2)$ or i or products of these. Applying an $SU(2)$ gate to the RHS of A does not change $A^{(2)}$, whereas applying i changes $A^{(2)}$ to its negative.

Now suppose $N_B = 3$. One can represent any $A \in SU(8)$ as

$$\begin{aligned} A = & e^{i\frac{\pi}{4}n(A)} \exp(ia_{jkr}\sigma_{X_jX_kX_r}) \\ & \exp(ia''_{jk}\sigma_{1X_jX_k}) \exp(ia'_{jk}\sigma_{X_j1X_k}) \exp(ia_{jk}\sigma_{X_jX_k1}) \\ & \exp(ia''_j\sigma_{X_j11}) \exp(ia'_j\sigma_{1X_j1}) \exp(ia_j\sigma_{11X_j}) . \end{aligned} \quad (18)$$

When the continuous parameters of A are small,

$$A^{(2)} \approx e^{i\frac{\pi}{2}n(A)} [1 + 2i(a''_{jk}\sigma_{1X_jX_k} + a'_{jk}\sigma_{X_j1X_k} + a_{jk}\sigma_{X_jX_k1})] . \quad (19)$$

This $A^{(2)}$ is independent of the a_{jkr} parameters. So, for $A, B \in SU(8)$, $A^{(2)} = \pm B^{(2)}$ or $A^{(2)} = \pm iB^{(2)}$ is a necessary but not a sufficient condition for $A \sim_R B$. More invariants than just $A^{(2)}$ are needed for $N_B > 2$.

Higher order invariants can be generated as follows. We will represent them diagrammatically using the symbols defined in Fig.2. Fig.3 shows second and fourth order invariants under LO-RHS for a circuit with 3 bits. The same idea can be used to generate invariants of order equal to any even number, for any number of qubits. Fig.4 explains why the circuits portrayed in Fig.3 are invariant under LO-RHS. Roughly speaking, if we apply a $U \in SU(2)$ to the RHS of $A \in SU(8)$, then, in the diagram of a fourth order invariant, a copy of U must be inserted next to each of the 4 copies of A . And these 4 copies of U annihilate each other. This paper will only use the second order invariant $A^{(2)}$. We will not even use Group Theory in this paper. For information on the group theoretic underpinnings of quantum circuit invariants, see, for example, Ref.[2].

$$A = \left(\begin{array}{c} \text{---} \\ \text{---} \\ \vdots \\ \text{---} \end{array} \right) \left(\begin{array}{c} \text{---} \\ \text{---} \\ \vdots \\ \text{---} \end{array} \right) \Bigg\}_{N_B} \quad A^T = \left(\begin{array}{c} \text{---} \\ \text{---} \\ \vdots \\ \text{---} \end{array} \right) \left(\begin{array}{c} \text{---} \\ \text{---} \\ \vdots \\ \text{---} \end{array} \right) \quad \sigma_Y = \bullet$$

Figure 2: Key to symbols used in Figs.3 and 4. $A \in SU(N_S)$.

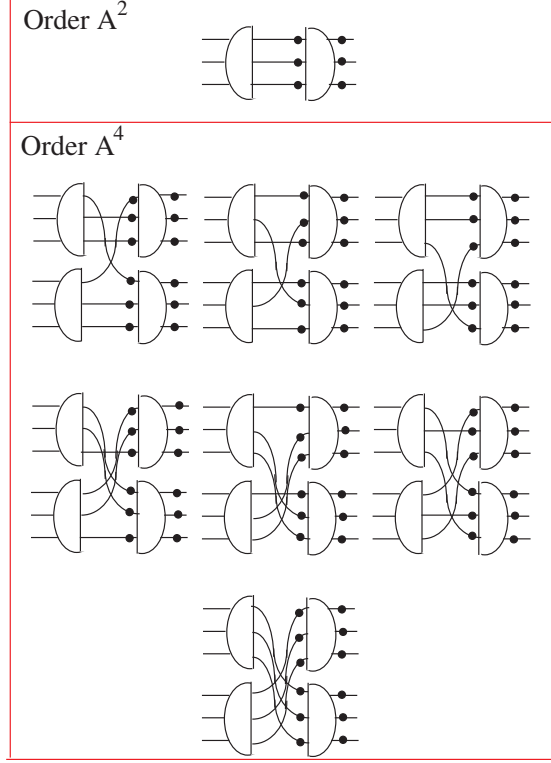


Figure 3: Second and fourth order invariants under LO-RHS for a circuit with 3 bits. $A \in SU(8)$.

4 Dressed CNOTs

[dr11.m, dr110.m, dr011.m, dr101.m,]

In this section, we define dressed CNOTs, a simple yet powerful generalization of the standard CNOT. We also discuss some simple properties of dressed CNOTs that will be used in subsequent sections.

The **controlled NOT (CNOT)** with control bit 1 and target bit 0, is defined by

$$\begin{array}{c} \text{---} \times \text{---} \\ | \\ \text{---} \bullet \text{---} \end{array} = (-1)^{n_X(0)n(1)} = \sigma_X(0)^{n(1)} . \quad (20)$$

Now suppose U and V are arbitrary elements of $SU(2)$. Define \hat{a} and \hat{a}' by $U\sigma_X U^\dagger = \sigma_{\hat{a}}$ and $V\sigma_Z V^\dagger = \sigma_{\hat{a}'}$. Then a **dressed CNOT (DC-NOT)** connecting bits 0 and

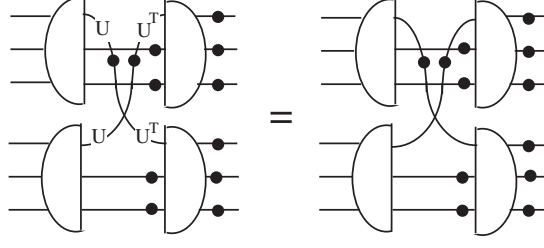


Figure 4: Why the diagrams shown in Fig.3 are invariant under LO-RHS. $A \in SU(8)$ and $U \in SU(2)$.

1, is defined by

$$\begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} = \begin{array}{c} \text{---} [U] \text{---} \times \text{---} [U^\dagger] \text{---} \\ | \\ \text{---} [V] \text{---} \bullet \text{---} [V^\dagger] \text{---} \end{array} = (-1)^{n_{\hat{a}}(0)n_{\hat{a}'}(1)} = \sigma_{\hat{a}}(0)^{n_{\hat{a}'}(1)} = \sigma_{\hat{a}'}(1)^{n_{\hat{a}}(0)} . \quad (21)$$

We will refer to the vectors \hat{a}' and \hat{a} as the **defining vectors** of the DC-NOT.

Sometimes in this paper, we will draw a circuit containing one or more DC-NOTs whose oval nodes are empty. By this we will mean that the omitted defining vectors are arbitrary and their precise value is unimportant in that context.

Consider the wire corresponding to bit μ in a quantum circuit. Within the bit- μ wire, consider two adjacent oval nodes belonging to two different DC-NOTs: $\text{---} \hat{a} \text{---} \hat{b} \text{---}$. If $\hat{b} \parallel \hat{a}$, we will say there is a **breach** at that position in the bit- μ wire. If $\hat{b} \perp \hat{a}$, we will say there is a **foil** at that position in the bit- μ wire.

Theorem 3

$$\begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} = \frac{1}{2}(1 + \sigma_{1,\hat{a}} + \sigma_{\hat{a}',1} - \sigma_{\hat{a}',\hat{a}}) . \quad (22)$$

proof:

$$\sigma_{\hat{a}'}(1)^{n_{\hat{a}}(0)} = \sigma_{\hat{a}'}(1)n_{\hat{a}}(0) + \bar{n}_{\hat{a}}(0) = \frac{1}{2}(1 + \sigma_{1,\hat{a}} + \sigma_{\hat{a}',1} - \sigma_{\hat{a}',\hat{a}}) . \quad (23)$$

QED

Theorem 4

$$\left(\begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} \right)^2 = 1 . \quad (24)$$

proof:

$$\sigma_{\hat{a}}(0)^{2n_{\hat{a}'}(1)} = 1.$$

QED

Theorem 5

$$\begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} = \begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \sigma_{\hat{a}'} \hat{a}' \text{---} \end{array} . \quad (25)$$

proof:

$$[-\sigma_{\hat{a}}(0)]^{n_{\hat{a}'}(1)} = (-1)^{n_{\hat{a}'}(1)} \sigma_{\hat{a}}(0)^{n_{\hat{a}'}(1)} = \sigma_{\hat{a}'}(1) \sigma_{\hat{a}}(0)^{n_{\hat{a}'}(1)} . \quad (26)$$

QED

In subsequent sections, we will often need to calculate the effect of a similarity transformation produced by pre and post multiplying an operator by the same DC-NOT. The next theorem will be useful for performing such calculations.

Theorem 6

$$\begin{array}{c} \text{---} \hat{b} \text{---} \sigma_{\vec{a}} \text{---} \hat{b} \text{---} \\ | \quad \quad | \\ \text{---} \hat{b}' \text{---} \quad \quad \text{---} \hat{b}' \text{---} \end{array} = \sigma_{1, \vec{a}_{\parallel \hat{b}}} + \sigma_{\hat{b}', \vec{a}_{\perp \hat{b}}} . \quad (27)$$

proof:

Clearly,

$$\begin{array}{c} \text{---} \hat{b} \text{---} \sigma_{\vec{a}_{\parallel \hat{b}}} \text{---} \hat{b} \text{---} \\ | \quad \quad | \\ \text{---} \hat{b}' \text{---} \quad \quad \text{---} \hat{b}' \text{---} \end{array} = \sigma_{1, \vec{a}_{\parallel \hat{b}}} . \quad (28)$$

On the other hand,

$$\begin{array}{c} \text{---} \hat{b} \text{---} \sigma_{\vec{a}_{\perp \hat{b}}} \text{---} \hat{b} \text{---} \\ | \quad \quad | \\ \text{---} \hat{b}' \text{---} \quad \quad \text{---} \hat{b}' \text{---} \end{array} = \begin{array}{c} \text{---} \sigma_{\vec{a}_{\perp \hat{b}}} \text{---} \hat{b} \text{---} \hat{b} \text{---} \\ | \quad \quad | \\ \text{---} \hat{b}' \text{---} \quad \quad \text{---} \hat{b}' \text{---} \end{array} = \sigma_{\hat{b}', \vec{a}_{\perp \hat{b}}} . \quad (29)$$

QED

5 Wake Identities

In this section we prove what we call a “wake identity”. We call it thus because in it, one DC-NOT is pushed through another, producing a third DC-NOT as its “wake”.

Theorem 7 Suppose $\hat{a}' \perp \hat{b}'$.

$$\begin{array}{c} \hat{b} \\ \downarrow \\ \hat{b}' \end{array} \begin{array}{c} \hat{a}' \\ \downarrow \\ \hat{a}'' \end{array} \perp = \begin{array}{c} \hat{b} \quad \hat{b} \\ \downarrow \quad \downarrow \\ \hat{a}' \quad \hat{b}' \\ \downarrow \quad \downarrow \\ \hat{a}'' \quad \hat{a}'' \end{array} \quad (30a)$$

$$= \begin{array}{c} \hat{b} \\ \downarrow \\ \hat{b}' \end{array} \begin{array}{c} \hat{a}' \\ \downarrow \\ \hat{a}'' \end{array} = \begin{array}{c} \hat{b} \quad \hat{b} \\ \downarrow \quad \downarrow \\ \hat{a}' \quad \hat{b}' \\ \downarrow \quad \downarrow \\ \hat{a}'' \quad \hat{a}'' \end{array} . \quad (30b)$$

proof:

$$\begin{array}{c} \hat{b} \\ \downarrow \\ \hat{b}' \end{array} \begin{array}{c} \hat{a}' \\ \downarrow \\ \hat{a}'' \end{array} \perp = \sigma_{\hat{a}'}(1)^{n_{\hat{a}''}(2)} \sigma_{\hat{b}'}(1)^{n_{\hat{b}}(0)} \sigma_{\hat{a}'}(1)^{n_{\hat{a}''}(2)} \quad (31a)$$

$$= [(-1)^{n_{\hat{a}''}(2)} \sigma_{\hat{b}'}(1)]^{n_{\hat{b}}(0)} \quad (31b)$$

$$= (-1)^{n_{\hat{a}''}(2)n_{\hat{b}}(0)} \sigma_{\hat{b}'}(1)^{n_{\hat{b}}(0)} \quad (31c)$$

$$= \begin{array}{c} \hat{b} \quad \hat{b} \\ \downarrow \quad \downarrow \\ \hat{b}' \\ \downarrow \\ \hat{a}'' \end{array} . \quad (31d)$$

QED

6 Swapper Identities

[swap_t3.m, test_swap_t3.m]

In this section, we discuss certain DC-NOT identities associated with the qubit Exchange Operator (a.k.a. Swap Operator or Swapper).

We will represent the Swapper by a double arrow connecting the two qubits being swapped. By definition, the Swapper satisfies

$$\begin{array}{c} \boxed{U} \\ \updownarrow \end{array} = \begin{array}{c} \updownarrow \\ \boxed{U} \end{array} \quad (32)$$

for any $U \in U(2)$. As is well known (for a proof, see, for example, Ref.[8]), the Swapper can be expressed as a product of 3 CNOTs:

$$\begin{array}{c} \updownarrow \\ \hline \end{array} = \begin{array}{c} \times \bullet \times \\ \times \bullet \times \end{array} . \quad (33)$$

The next theorem shows that the Swapper can also be expressed as a product of 3 DC-NOTs.

Theorem 8 Suppose $\hat{a} \perp \hat{b}$, $U \in SU(2)$, $U^\dagger \sigma_{\hat{a}} U = \sigma_{\hat{a}'}$, and $U^\dagger \sigma_{\hat{b}} U = \sigma_{\hat{b}'}$.

$$\begin{array}{c} \updownarrow \\ \hline \end{array} = \begin{array}{c} \hat{a} \perp \hat{b} \perp \hat{a} \\ | \quad | \quad | \\ \hat{b} \perp \hat{a} \perp \hat{b} \end{array} \quad (34a)$$

$$= \begin{array}{c} \hat{a} \perp \hat{b} \perp \hat{a} \quad U \\ | \quad | \quad | \\ \hat{b}' \perp \hat{a}' \perp \hat{b}' \quad U^\dagger \end{array} . \quad (34b)$$

proof:

Since $\hat{a} \perp \hat{b}$, there exists $V \in SU(2)$ such that $V^\dagger \sigma_X V = \sigma_{\hat{a}}$ and $V^\dagger \sigma_Z V = \sigma_{\hat{b}}$. Then

$$\begin{array}{c} \updownarrow \\ \hline \end{array} = \begin{array}{c} \boxed{V^\dagger} \updownarrow \boxed{V} \\ \boxed{V^\dagger} \updownarrow \boxed{V} \end{array} = \begin{array}{c} \boxed{V^\dagger} \times \bullet \times \boxed{V} \\ \boxed{V^\dagger} \bullet \times \bullet \boxed{V} \end{array} = \begin{array}{c} \hat{a} \hat{b} \hat{a} \\ | \quad | \quad | \\ \hat{b} \hat{a} \hat{b} \end{array} . \quad (35)$$

This proves Eq.(34a). Eq.(34b) follows from

$$\begin{array}{c} \updownarrow \\ \hline \end{array} = \begin{array}{c} \updownarrow \quad \boxed{U} \\ \boxed{U^\dagger} \updownarrow \boxed{U} \quad \boxed{U^\dagger} \end{array} . \quad (36)$$

QED

We will refer to the next identity, Eq.(37), as the 2/3-Swapper identity, because its LHS contains 2/3 of a Swapper.

Theorem 9 For any $\alpha \in \mathbb{R}$,

$$\begin{array}{c} \hat{x} \hat{z} \\ | \quad | \\ \hat{x} \hat{z} \end{array} = \begin{array}{c} \hat{q}_{xy} \hat{z} \quad U \\ | \quad | \\ \hat{q}'_{xy} \hat{z} \quad U' \end{array} \quad (37a)$$

$$= \begin{array}{c} U \hat{x} \hat{p}'_{zy} \\ | \quad | \\ U' \hat{x} \hat{p}_{zy} \end{array} , \quad (37b)$$

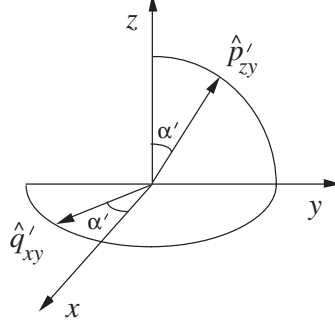


Figure 5: Orientation of vectors \hat{q}'_{xy} and \hat{p}'_{zy} . Note that $H\sigma_{\hat{p}'_{zy}}H = \sigma_{\hat{q}'_{xy}}$. The same picture, but omitting all primes, describes \hat{q}_{xy} and \hat{p}_{zy} .

where (see Fig.5)

$$\hat{p}_{zy} = c_\alpha \hat{z} + s_\alpha \hat{y} , \quad \hat{p}'_{zy} = (\hat{p}_{zy})_{\alpha \rightarrow \alpha'} , \quad (38)$$

$$\hat{q}_{xy} = c_\alpha \hat{x} - s_\alpha \hat{y} , \quad \hat{q}'_{xy} = (\hat{q}_{xy})_{\alpha \rightarrow \alpha'} , \quad (39)$$

(p vector has a positive sign in front of s_α , q vector has a negative one) and

$$U = e^{i\frac{\alpha}{2}\sigma_z} e^{-i\frac{\alpha'}{2}\sigma_x} , \quad U' = (U)_{\alpha \leftrightarrow \alpha'} . \quad (40)$$

Note that the left-hand sides of Eqs.(37a) and (37b) are independent of the two angles α and α' ; only their right-hand sides depend on these angles.

proof:

From the expression of Swapper as a product of 3 CNOTs, we get

$$\begin{array}{c} \text{---} \hat{z} \text{---} \hat{x} \text{---} \hat{z} \text{---} \\ | \quad | \quad | \\ \text{---} \hat{z} \text{---} \hat{x} \text{---} \hat{z} \text{---} \end{array} = \begin{array}{c} \updownarrow \boxed{H} \text{---} \\ \updownarrow \boxed{H} \text{---} \end{array} . \quad (41)$$

From Fig.5, it follows that

$$\sigma_{\hat{q}_{xy}} = e^{i\frac{\alpha}{2}\sigma_z} \sigma_{\hat{x}} e^{-i\frac{\alpha}{2}\sigma_z} . \quad (42)$$

Thus

$$\begin{array}{c}
 \begin{array}{c} \hat{z} \quad \hat{q}_{xy} \quad \hat{x} \quad \hat{z} \\ \hat{z} \quad \hat{q}'_{xy} \quad \hat{x} \quad \hat{z} \end{array} = \begin{array}{c} \hat{z} \quad \hat{q}_{xy} \quad \hat{z} \\ \hat{z} \quad \hat{q}'_{xy} \quad \hat{z} \end{array} \begin{array}{c} \uparrow \\ \downarrow \end{array} \begin{array}{c} H \\ H \end{array} \\
 \end{array} \quad (43a)$$

$$\begin{array}{c}
 \begin{array}{c} e^{i\frac{\alpha}{2}\sigma_z} \quad \hat{z} \quad \hat{x} \quad \hat{z} \quad e^{-i\frac{\alpha}{2}\sigma_z} \\ e^{i\frac{\alpha'}{2}\sigma_z} \quad \hat{z} \quad \hat{x} \quad \hat{z} \quad e^{-i\frac{\alpha'}{2}\sigma_z} \end{array} \begin{array}{c} \uparrow \\ \downarrow \end{array} \begin{array}{c} H \\ H \end{array} \\
 = \\
 \end{array} \quad (43b)$$

$$\begin{array}{c}
 \begin{array}{c} e^{i\frac{\alpha}{2}\sigma_z} \quad \uparrow \quad H \quad e^{-i\frac{\alpha}{2}\sigma_z} \quad \uparrow \quad H \\ e^{i\frac{\alpha'}{2}\sigma_z} \quad \downarrow \quad H \quad e^{-i\frac{\alpha'}{2}\sigma_z} \quad \downarrow \quad H \end{array} \\
 = \\
 \end{array} \quad (43c)$$

$$\begin{array}{c}
 \begin{array}{c} e^{i\frac{\alpha}{2}\sigma_z} e^{-i\frac{\alpha'}{2}\sigma_x} \\ e^{i\frac{\alpha'}{2}\sigma_z} e^{-i\frac{\alpha}{2}\sigma_x} \end{array} \\
 = \\
 \end{array} . \quad (43d)$$

QED

The next theorem follows immediately from the previous one, by a change of basis.

Theorem 10 Suppose $\alpha \in \mathbb{R}$, $\hat{a} \perp \hat{b}$, and $\hat{a}' \perp \hat{b}'$. Then

$$\begin{array}{c}
 \begin{array}{c} \hat{b} \quad \hat{a} \\ \hat{b}' \quad \hat{a}' \end{array} \begin{array}{c} \perp \\ \perp \end{array} = \begin{array}{c} \hat{b}_f \quad \hat{a} \quad U \\ \hat{b}'_f \quad \hat{a}' \quad U' \end{array} \\
 \end{array} \quad (44a)$$

$$\begin{array}{c}
 \begin{array}{c} U \quad \hat{b} \quad \hat{a}'_f \\ U' \quad \hat{b}' \quad \hat{a}_f \end{array} \begin{array}{c} \perp \\ \perp \end{array} , \\
 = \\
 \end{array} \quad (44b)$$

where

$$\hat{a}_f = c_\alpha \hat{a} + s_\alpha [\hat{a}\hat{b}] , \quad \hat{a}'_f = c_{\alpha'} \hat{a}' + s_{\alpha'} [\hat{a}'\hat{b}'] , \quad (45)$$

$$\hat{b}_f = c_\alpha \hat{b} - s_\alpha [\hat{a}\hat{b}] , \quad \hat{b}'_f = c_{\alpha'} \hat{b}' - s_{\alpha'} [\hat{a}'\hat{b}'] , \quad (46)$$

and

$$U = e^{i\frac{\alpha}{2}\sigma_{\hat{a}}} e^{-i\frac{\alpha}{2}\sigma_{\hat{b}}} , \quad U' = e^{i\frac{\alpha'}{2}\sigma_{\hat{a}'}} e^{-i\frac{\alpha'}{2}\sigma_{\hat{b}'}} . \quad (47)$$

proof:

Just change basis in the space where bit 0 (ditto, bit 1) lives so that $(\hat{x}, \hat{y}, \hat{z})$ is replaced by $(\hat{b}, [\hat{a}\hat{b}], \hat{a})$ (ditto, $(\hat{b}', [\hat{a}'\hat{b}'], \hat{a}')$).

QED

We will refer to the next identity, Eq.(48), as the 1/3 Swapper identity.

Theorem 11

$$\begin{array}{c} \text{---} \hat{x} \text{---} \hat{q}_{xy} \text{---} \\ | \\ \text{---} \hat{x} \text{---} \hat{q}'_{xy} \text{---} \end{array} = \begin{array}{c} \text{---} \hat{z} \text{---} \hat{p}'_{zy} \text{---} U^\dagger \\ | \\ \text{---} \hat{z} \text{---} \hat{p}_{zy} \text{---} U'^\dagger \end{array}, \quad (48)$$

where all variables are defined as in Theorem 9.

proof:

From the Hermitian conjugate of Eq.(37a), one gets

$$\begin{array}{c} \text{---} \hat{z} \text{---} \hat{x} \text{---} \hat{q}_{xy} \text{---} \\ | \\ \text{---} \hat{z} \text{---} \hat{x} \text{---} \hat{q}'_{xy} \text{---} \end{array} = \begin{array}{c} \text{---} U^\dagger \text{---} \hat{z} \text{---} \\ | \\ \text{---} U'^\dagger \text{---} \hat{z} \text{---} \end{array}. \quad (49)$$

Let *LHS* and *RHS* stand for the left and right hand sides of Eq.(48). Pre-multiplying

both sides of the last equation by $\begin{array}{c} \hat{z} \\ | \\ \hat{z} \end{array}$ yields

$$\begin{array}{c} \hat{z} \\ | \\ \hat{z} \end{array} \begin{array}{c} \text{---} \hat{z} \text{---} \hat{x} \text{---} \hat{q}_{xy} \text{---} \\ | \\ \text{---} \hat{z} \text{---} \hat{x} \text{---} \hat{q}'_{xy} \text{---} \end{array} = \begin{array}{c} \text{---} U^\dagger \text{---} \hat{z} \text{---} \\ | \\ \text{---} U'^\dagger \text{---} \hat{z} \text{---} \end{array} \begin{array}{c} \hat{z} \\ | \\ \hat{z} \end{array} = RHS. \quad (50)$$

QED

7 DC-NOT Similarity Transformation Identities

[sim_trans_t4.m, test_sim_trans_t4.m]

In this section, we present some identities which contain a similarity transformation produced by pre and post multiplying an operator by the same DC-NOT.

We will refer to the next theorem as the DC-NOT similarity transformation identity.

Theorem 12 For any $\alpha, \lambda \in \mathbb{R}$,

$$\begin{array}{c} \text{---} \hat{x} \text{---} [c_\alpha \sigma_X + s_\alpha \sigma_Z] \text{---} \hat{x} \text{---} \\ | \\ \text{---} \hat{x} \text{---} [s_\alpha \sigma_X + c_\alpha \sigma_Z] \text{---} \hat{x} \text{---} \end{array} = \begin{array}{c} \text{---} \hat{q}_{xy} \text{---} [c_\alpha \sigma_{\hat{q}_{xy}} + s_\alpha \sigma_Z] \text{---} \hat{q}_{xy} \text{---} \\ | \\ \text{---} \hat{q}_{xy} \text{---} [s_\alpha \sigma_{\hat{q}_{xy}} + c_\alpha \sigma_Z] \text{---} \hat{q}_{xy} \text{---} \end{array}, \quad (51)$$

where $\hat{q}_{xy} = c_\lambda \hat{x} - s_\lambda \hat{y}$. Note that the LHS of Eq.(51) equals its RHS evaluated at $\lambda = 0$.

proof:

Since

$$[\hat{q}_{xy}\hat{z}] = -(c_\lambda \hat{y} + s_\lambda \hat{x}) , \quad (52)$$

it follows that

$$\sigma_{\hat{q}_{xy}\hat{q}_{xy}} + \sigma_{[\hat{q}_{xy}\hat{z}][\hat{q}_{xy}\hat{z}]} = \sigma_{c_\lambda \hat{x} - s_\lambda \hat{y}, c_\lambda \hat{x} - s_\lambda \hat{y}} + \sigma_{c_\lambda \hat{y} + s_\lambda \hat{x}, c_\lambda \hat{y} + s_\lambda \hat{x}} \quad (53a)$$

$$= \sigma_{\hat{x}\hat{x}} + \sigma_{\hat{y}\hat{y}} . \quad (53b)$$

Let LHS and RHS denote the left-hand side and right-hand side, respectively, of Eq.(51). Then, using Eq.(27),

$$RHS = \begin{array}{ccc} \begin{array}{c} \textcircled{\hat{q}_{xy}} \\ | \\ \textcircled{\hat{q}_{xy}} \end{array} & (s_\alpha \sigma_{\hat{q}_{xy},1} + c_\alpha \sigma_{\hat{z},1}) & \begin{array}{c} \textcircled{\hat{q}_{xy}} \\ | \\ \textcircled{\hat{q}_{xy}} \end{array} \quad \begin{array}{c} \textcircled{\hat{q}_{xy}} \\ | \\ \textcircled{\hat{q}_{xy}} \end{array} (c_\alpha \sigma_{1,\hat{q}_{xy}} + s_\alpha \sigma_{1,\hat{z}}) \quad \begin{array}{c} \textcircled{\hat{q}_{xy}} \\ | \\ \textcircled{\hat{q}_{xy}} \end{array} \end{array} \quad (54a)$$

$$= (s_\alpha \sigma_{\hat{q}_{xy},1} + c_\alpha \sigma_{\hat{z},1}) (c_\alpha \sigma_{1,\hat{q}_{xy}} + s_\alpha \sigma_{1,\hat{z}}) \quad (54b)$$

$$= s_\alpha c_\alpha (\sigma_{\hat{q}_{xy}\hat{q}_{xy}} + \sigma_{[\hat{q}_{xy}\hat{z}][\hat{q}_{xy}\hat{z}]}) + c_\alpha^2 \sigma_{\hat{z},1} + s_\alpha^2 \sigma_{1,\hat{z}} \quad (54c)$$

$$= s_\alpha c_\alpha (\sigma_{\hat{x}\hat{x}} + \sigma_{\hat{y}\hat{y}}) + c_\alpha^2 \sigma_{\hat{z},1} + s_\alpha^2 \sigma_{1,\hat{z}} \quad (54d)$$

$$= LHS . \quad (54e)$$

QED

It is convenient to define, for any $\xi \in \mathbb{R}$,

$$\hat{p}_{w_1,w_2}^\xi = c_\xi \hat{w}_1 + s_\xi \hat{w}_2 , \quad \hat{q}_{w_1,w_2}^\xi = c_\xi \hat{w}_1 - s_\xi \hat{w}_2 . \quad (55)$$

(The \hat{p} vectors have a positive sign in front of the sine function whereas the \hat{q} vectors have a negative one).

The next theorem follows from the DC-NOT similarity transformation identity.

Theorem 13 For any $\phi, \lambda \in \mathbb{R}$,

$$\begin{array}{ccccc} \text{---} \textcircled{\hat{p}_{zx}^\phi} \text{---} \textcircled{\hat{x}} \text{---} \textcircled{\hat{q}_{xy}^\lambda} \text{---} & & \text{---} \textcircled{\hat{a}_f} \text{---} \boxed{U} \text{---} \\ | & & | \\ \text{---} \textcircled{\hat{q}_{zx}^\phi} \text{---} \textcircled{\hat{x}} \text{---} \textcircled{\hat{q}_{xy}^\lambda} \text{---} & = & \text{---} \textcircled{\hat{a}'_f} \text{---} \boxed{U'} \text{---} \end{array} , \quad (56)$$

where (see Fig.6)

$$\hat{a}_f = c_\lambda \hat{p}_{zx}^\phi + s_\lambda \hat{y} , \quad \hat{a}'_f = c_\lambda \hat{q}_{zx}^\phi + s_\lambda \hat{y} , \quad (57)$$

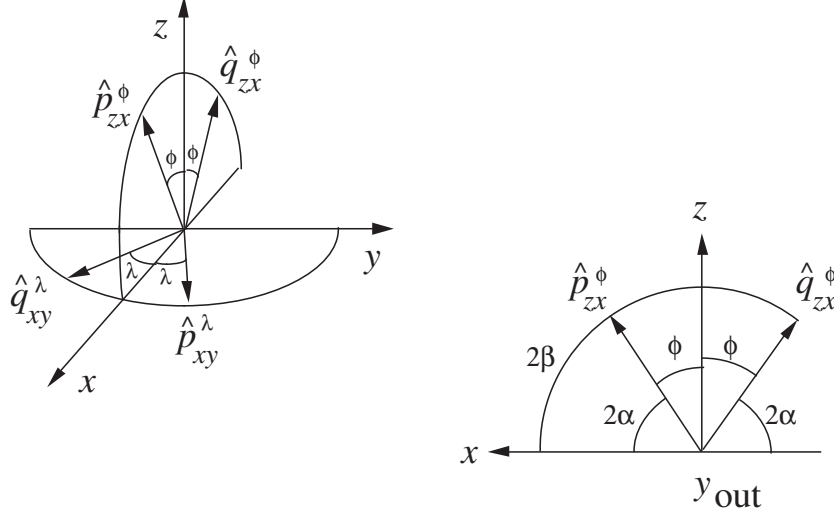


Figure 6: Variables used in Theorem 13.

and

$$U = (c_\alpha \sigma_X + s_\alpha \sigma_Z)(c_\alpha \sigma_{\hat{q}_{xy}^\lambda} + s_\alpha \sigma_Z), \quad U' = (U)_{\alpha \rightarrow \beta}, \quad (58)$$

where

$$2\alpha = \frac{\pi}{2} - \phi, \quad 2\beta = \pi - 2\alpha. \quad (59)$$

proof:

From Fig.6, it follows that

$$\hat{p}_{zx}^\phi = e^{i\alpha\sigma_Y} \sigma_X e^{-i\alpha\sigma_Y}, \quad (60)$$

and

$$\hat{q}_{zx}^\phi = e^{i\beta\sigma_Y} \sigma_X e^{-i\beta\sigma_Y}. \quad (61)$$

Let LHS and RHS denote the left-hand side and right-hand side, respectively, of Eq.(56). Then

$$LHS = \begin{array}{c} \text{---} \boxed{e^{i\alpha\sigma_Y}} \text{---} \hat{x} \text{---} \boxed{e^{-i\alpha\sigma_Y}} \text{---} \hat{x} \text{---} \hat{q}_{xy}^\lambda \text{---} \\ \text{---} \boxed{e^{i\beta\sigma_Y}} \text{---} \hat{x} \text{---} \boxed{e^{-i\beta\sigma_Y}} \text{---} \hat{x} \text{---} \hat{q}_{xy}^\lambda \text{---} \end{array}, \quad (62)$$

and

$$RHS = \begin{array}{c} \text{---} [e^{i\alpha\sigma_Y}] \text{---} \hat{p}_{xy}^\lambda \text{---} [e^{-i\alpha\sigma_Y}] \text{---} U \text{---} \\ | \\ \text{---} [e^{i\beta\sigma_Y}] \text{---} \hat{p}_{xy}^\lambda \text{---} [e^{-i\beta\sigma_Y}] \text{---} U' \text{---} \end{array} \quad (63)$$

Therefore, Eq.(56) is equivalent to the assertion that

$$\begin{array}{c} \hat{x} \text{---} [e^{-i\alpha\sigma_Y}] \text{---} \hat{x} \\ | \\ \hat{x} \text{---} [e^{-i\beta\sigma_Y}] \text{---} \hat{x} \end{array} = \begin{array}{c} \hat{p}_{xy}^\lambda \text{---} [e^{-i\alpha\sigma_Y} U] \text{---} \hat{q}_{xy}^\lambda \\ | \\ \hat{p}_{xy}^\lambda \text{---} [e^{-i\beta\sigma_Y} U'] \text{---} \hat{q}_{xy}^\lambda \end{array} \quad (64)$$

Now pre-multiply each side of the last equation by σ_{XX}

$$\begin{array}{c} \hat{x} \text{---} [c_\alpha \sigma_X + s_\alpha \sigma_Z] \text{---} \hat{x} \\ | \\ \hat{x} \text{---} [c_\beta \sigma_X + s_\beta \sigma_Z] \text{---} \hat{x} \end{array} = \begin{array}{c} \hat{q}_{xy}^\lambda \text{---} [c_\alpha \sigma_{\hat{q}_{xy}^\lambda} + s_\alpha \sigma_Z] \text{---} \hat{q}_{xy}^\lambda \\ | \\ \hat{q}_{xy}^\lambda \text{---} [c_\beta \sigma_{\hat{q}_{xy}^\lambda} + s_\beta \sigma_Z] \text{---} \hat{q}_{xy}^\lambda \end{array} \quad (65)$$

The preceding equation follows from Theorem 12 and the fact that $\alpha + \beta = \pi/2$.

QED

The next theorem is a simple variation of the previous one. (The left-hand sides of Eqs.(56) and (66) differ only in that one circuit has two q 's in the bit-1 wire whereas the other circuit has two p 's.)

Theorem 14

$$\begin{array}{c} \hat{p}_{zx}^\phi \text{---} \hat{x} \text{---} \hat{q}_{xy}^\lambda \\ | \\ \hat{p}_{zx}^\phi \text{---} \hat{x} \text{---} \hat{p}_{xy}^\lambda \end{array} = \begin{array}{c} [\sigma_Z] \text{---} \hat{a}'_f \text{---} [U' \sigma_Z] \\ | \\ \hat{a}_f \text{---} [U \sigma_{\hat{q}_{xy}^\lambda} \sigma_X] \end{array}, \quad (66)$$

where all variables are defined as in Theorem 13.

proof:

Let LHS_{56} represent the left-hand side of Eq.(56), and LHS_{66} , the left-hand side of Eq.(66). Then

$$\begin{array}{c} \text{---} \\ | \\ \text{---} [\sigma_Z] \text{---} \end{array} LHS_{56} \begin{array}{c} \text{---} [\sigma_{\hat{q}_{xy}^\lambda} \sigma_X] \text{---} \\ | \\ \text{---} [\sigma_Z] \text{---} \end{array} = \begin{array}{c} \hat{p}_{zx}^\phi \text{---} \hat{x} \text{---} \hat{q}_{xy}^\lambda \text{---} [\sigma_{\hat{q}_{xy}^\lambda} \sigma_X] \\ | \\ \hat{p}_{zx}^\phi \text{---} -\hat{x} \text{---} -\hat{q}_{xy}^\lambda \end{array} \quad (67a)$$

$$= \begin{array}{c} \hat{p}_{zx}^\phi \text{---} \hat{x} \text{---} [\sigma_X] \text{---} \hat{q}_{xy}^\lambda \text{---} [(\sigma_{\hat{q}_{xy}^\lambda})^2 \sigma_X] \\ | \\ \hat{p}_{zx}^\phi \text{---} \hat{x} \text{---} \hat{q}_{xy}^\lambda \end{array} \quad (67b)$$

$$= \begin{array}{c} \updownarrow \\ \text{---} LHS_{66} \text{---} \\ \updownarrow \end{array} \quad (67c)$$

The right-hand sides of Eqs.(56) and (66) must be related in the same way as their left-hand sides.

QED

8 LO-RHS Invariant for Circuits with Two Qubits, and Multiple DC-NOTs

In previous sections we defined the LO-RHS invariant $A^{(2)}$ for any $A \in U(N_S)$. We also defined DC-NOTs and discussed some of their properties. In this section, we combine these two concepts: we calculate $A^{(2)}$ when A is a product of one or more DC-NOTs acting on the same two qubits.

Henceforth, we will denote the product of r DC-NOTs (all acting on the same two qubits) by the symbol \mathcal{G}_r followed by a list (enclosed in parenthesis) of its arguments. Sometimes, if this doesn't lead to confusion, its list of arguments will be omitted. Thus,

$$\mathcal{G}_r \left(\begin{array}{cccc} \hat{a}_r & \cdots & \hat{a}_2 & \hat{a}_1 \\ \hat{a}'_r & \cdots & \hat{a}'_2 & \hat{a}'_1 \end{array} \right) = \begin{array}{c} \text{---} \hat{a}_r \text{---} \\ | \\ \text{---} \hat{a}'_r \text{---} \end{array} \cdots \begin{array}{c} \text{---} \hat{a}_2 \text{---} \hat{a}_1 \text{---} \\ | \quad | \\ \text{---} \hat{a}'_2 \text{---} \hat{a}'_1 \text{---} \end{array} . \quad (68)$$

The determinant of \mathcal{G}_r equals either plus or minus one. Indeed,

$$\det \left(\begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} \right) = \det \left(\begin{array}{c} \text{---} \text{---} \\ | \quad \text{---} \\ \text{---} \end{array} \right) = \det \begin{bmatrix} I_2 & 0 \\ 0 & \sigma_X \end{bmatrix} = -1 . \quad (69)$$

Since $\det(AB) = \det(A)\det(B)$, it follows that for $r = \mathbb{Z}^{>0}$,

$$\det(\mathcal{G}_r) = (-1)^r . \quad (70)$$

It is convenient to define a matrix $\hat{\mathcal{G}}_r$ by

$$\hat{\mathcal{G}}_r = (-1)^{\frac{r}{4}} \mathcal{G}_r = i^{\frac{r}{2}} \mathcal{G}_r . \quad (71)$$

Henceforth, we will refer to $\hat{\mathcal{G}}_r$ as the **special counterpart** of \mathcal{G}_r . (Here the adjective “special” means “having unit determinant”). $\hat{\mathcal{G}}_r \in U(4)$ and $\det(\hat{\mathcal{G}}_r) = 1$, so $\hat{\mathcal{G}}_r \in SU(4)$.

Since $\sigma_Y \sigma_a^T \sigma_Y = \sigma_{-\hat{a}}$,

$$\mathcal{G}_r^{(2)} = \mathcal{G}_r \sigma_{YY} \mathcal{G}_r^T \sigma_{YY} \quad (72a)$$

$$= \begin{array}{c} \text{---} \hat{a}_r \text{---} \\ | \\ \text{---} \hat{a}'_r \text{---} \end{array} \cdots \begin{array}{c} \text{---} \hat{a}_2 \text{---} \hat{a}_1 \text{---} -\hat{a}_1 \text{---} -\hat{a}_2 \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \hat{a}'_2 \text{---} \hat{a}'_1 \text{---} -\hat{a}'_1 \text{---} -\hat{a}'_2 \text{---} \end{array} \cdots \begin{array}{c} \text{---} -\hat{a}_r \text{---} \\ | \\ \text{---} -\hat{a}'_r \text{---} \end{array} . \quad (72b)$$

For $r \in \mathbb{Z}^{>0}$, $\mathcal{G}_r^{(2)}$ obeys the following recursion relation:

$$\mathcal{G}_{r+1}^{(2)} = \begin{array}{c} \text{---} \hat{a}_{r+1} \text{---} \\ | \\ \text{---} \hat{a}'_{r+1} \text{---} \end{array} \mathcal{G}_r^{(2)} \begin{array}{c} \text{---} -\hat{a}_{r+1} \text{---} \\ | \\ \text{---} -\hat{a}'_{r+1} \text{---} \end{array} . \quad (73)$$

Note that the LO-RHS invariants of \mathcal{G}_r and of its special counterpart $\hat{\mathcal{G}}_r$ are related by

$$\hat{\mathcal{G}}_r^{(2)} = i^r \mathcal{G}_r^{(2)} . \quad (74)$$

The remainder of Section 8 consists of 4 subsections which give explicit formulas for $\mathcal{G}_r^{(2)}$ for r from 1 to 4. These 4 subsections are very useful, but make for dry reading when considered in isolation; they only come alive and prove their mettle as we start using them in subsequent sections. Thus, the reader is advised not to spend too much time on them during his first reading of this paper. He should skim the 4 subsections, and then come back to them as the need arises.

8.1 Invariant for Circuits with 1 DC-NOT

[ckt_invar123.m]

This part of our program is dedicated to the letters $\mathcal{G}_1^{(2)}$.

Theorem 15

$$\mathcal{G}_1^{(2)} = \begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} \begin{array}{c} \text{---} -\hat{a} \text{---} \\ | \\ \text{---} -\hat{a}' \text{---} \end{array} = -\sigma_{\hat{a}', \hat{a}} . \quad (75)$$

proof:

$$\begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} \begin{array}{c} \text{---} -\hat{a} \text{---} \\ | \\ \text{---} -\hat{a}' \text{---} \end{array} = \begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \end{array} \begin{array}{c} \text{---} -\hat{a} \text{---} \end{array} \begin{array}{c} \boxed{\sigma_{-\hat{a}}} \\ \text{---} \end{array} = \begin{array}{c} \boxed{\sigma_{-\hat{a}}} \\ \boxed{\sigma_{\hat{a}'}} \end{array} . \quad (76)$$

QED

8.2 Invariant for Circuits with 2 DC-NOTs

[ckt_invar123.m, diag_ckt_invar2.m, diag_ckt_invar2_aux.m,
test_diag_invar2.m]

This part of our program is dedicated to the letters $\mathcal{G}_2^{(2)}$.

Theorem 16

$$\mathcal{G}_2^{(2)} = \begin{array}{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} -\hat{a} \text{---} -\hat{b} \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \hat{b}' \text{---} \hat{a}' \text{---} -\hat{a}' \text{---} -\hat{b}' \text{---} \end{array} \quad (77a)$$

$$= \lambda_{2r} + i\lambda_{2i} + \Lambda_{2r} + i\Lambda_{2i} , \quad (77b)$$

where

$$\lambda_{2r} = (\hat{a} \cdot \hat{b})(\hat{a}' \cdot \hat{b}') , \quad (78)$$

$$\lambda_{2i} = 0 , \quad (79)$$

$$\Lambda_{2r} = -\sigma_{[\hat{a}'\hat{b}'\hat{b}'], [\hat{a}\hat{b}\hat{b}]} , \quad (80)$$

$$\Lambda_{2i} = \hat{a} \cdot \hat{b} \sigma_{\hat{a}' \times \hat{b}', \hat{b}} + \hat{a}' \cdot \hat{b}' \sigma_{\hat{b}', \hat{a} \times \hat{b}} . \quad (81)$$

proof:

An explicit expression for $\mathcal{G}_1^{(2)}$ was given in Section 8.1. Eq.(27) shows how to calculate the effect of DC-NOT similarity transformations. Using these two results, one gets

$$\mathcal{G}_2^{(2)} = \begin{array}{c} \hat{b} \\ | \\ \hat{b}' \end{array} \begin{array}{c} [-\sigma_{\hat{a}', \hat{a}}] \\ \hat{b} \\ | \\ -\hat{b}' \end{array} \quad (82a)$$

$$= \begin{array}{c} \hat{b} \\ | \\ \hat{b}' \end{array} \begin{array}{c} \sigma_{\hat{a}', 1} \\ \hat{b} \\ | \\ \hat{b}' \end{array} \begin{array}{c} \hat{b} \\ | \\ \hat{b}' \end{array} \begin{array}{c} \sigma_{1, \hat{a}} \\ \hat{b} \\ | \\ \hat{b}' \end{array} \begin{array}{c} \hat{b} \\ | \\ \hat{b}' \end{array} \begin{array}{c} \hat{b} \\ | \\ \hat{b}' \end{array} \begin{array}{c} -\hat{b} \\ | \\ -\hat{b}' \end{array} (-1) \quad (82b)$$

$$= (\sigma_{\hat{a}'_{\parallel \hat{b}'}, 1} + \sigma_{\hat{a}'_{\perp \hat{b}'}, \hat{b}})(\sigma_{1, \hat{a}_{\parallel \hat{b}}} + \sigma_{\hat{b}, \hat{a}_{\perp \hat{b}}})\sigma_{\hat{b}', \hat{b}} \quad (82c)$$

$$= \begin{cases} (\hat{a}' \cdot \hat{b}')(\hat{a} \cdot \hat{b}) \\ -\sigma_{[\hat{a}'\hat{b}'\hat{b}'], [\hat{a}\hat{b}\hat{b}]} \\ +i \left[\hat{a} \cdot \hat{b} \sigma_{\hat{a}' \times \hat{b}', \hat{b}} + \hat{a}' \cdot \hat{b}' \sigma_{\hat{b}', \hat{a} \times \hat{b}} \right] \end{cases} . \quad (82d)$$

QED

Theorem 17

$$[\Lambda_{2r}, \Lambda_{2i}] = 0 , \quad (83)$$

$$(\Lambda_{2r}^\Gamma)^T \Lambda_{2i}^\Gamma = 0 , \quad (84)$$

$$\Lambda_{2r}^\Gamma (\Lambda_{2i}^\Gamma)^T = 0 . \quad (85)$$

proof:

This follows easily from Eqs.(80) and (81).

QED

It is convenient to parameterize the expression for $\mathcal{G}_2^{(2)}$ given by Theorem 16, using as few parameters as possible.

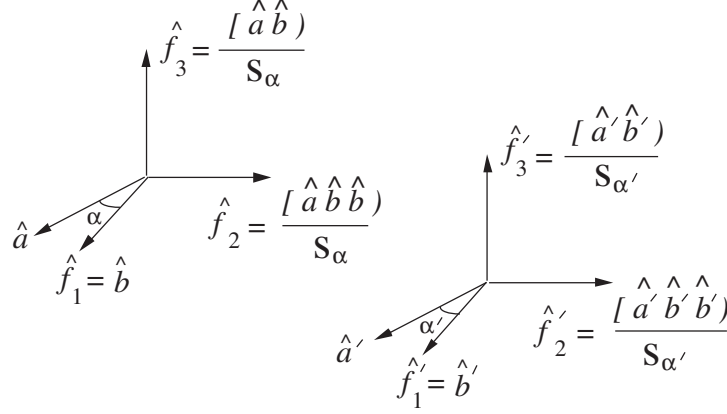


Figure 7: Principal parameters of $\mathcal{G}_2^{(2)}$.

Theorem 18 $\mathcal{G}_2^{(2)}$ can be parameterized with 2 real numbers α, α' , and 2 RHON bases $(\hat{f}_j)_{j=1,2,3}$ and $(\hat{f}'_j)_{j=1,2,3}$. Call these the principal parameters of $\mathcal{G}_2^{(2)}$ (see Fig.7). More explicitly,

$$\mathcal{G}_2^{(2)} = \lambda_{2r} + \Lambda_{2r} + i\Lambda_{2i} , \quad (86)$$

where

$$\lambda_{2r} = c_{\alpha'} c_{\alpha} , \quad (87)$$

$$\Lambda_{2r} = -(s_{\alpha'} s_{\alpha}) \hat{f}'_2 \hat{f}_2^T , \quad (88)$$

$$\Lambda_{2i} = (s_{\alpha'} c_{\alpha}) \hat{f}'_3 \hat{f}_1^T + (c_{\alpha'} s_{\alpha}) \hat{f}'_1 \hat{f}_3^T \quad (89a)$$

$$= \begin{array}{c|cc} & \hat{f}_1^T & \hat{f}_3^T \\ \hline \hat{f}'_3 & s_{\alpha'} c_{\alpha} & 0 \\ \hat{f}'_1 & 0 & c_{\alpha'} s_{\alpha} \end{array} \quad (89b)$$

$$= \begin{bmatrix} \hat{f}'_3 & \hat{f}'_1 \end{bmatrix} \begin{bmatrix} s_{\alpha'} c_{\alpha} & 0 \\ 0 & c_{\alpha'} s_{\alpha} \end{bmatrix} \begin{bmatrix} \hat{f}_1 & \hat{f}_3 \end{bmatrix}^T . \quad (89c)$$

(Eqs.(89a), (89b), and (89c) are 3 different styles of representing the same thing.)

proof:

Define $\alpha' \in [0, \pi)$ to be the angle between \hat{a}' and \hat{b}' . Thus

$$c_{\alpha'} = \hat{a}' \cdot \hat{b}' , \quad s_{\alpha'} = |\hat{a}' \times \hat{b}'| . \quad (90)$$

If $s_{\alpha'} \neq 0$, set

$$(f'_j)_{j=1,2,3} = (\hat{b}', \frac{[\hat{a}'\hat{b}'\hat{b}']}{s_{\alpha'}}, \frac{[\hat{a}'\hat{b}']}{s_{\alpha'}}) . \quad (91)$$

If $s_{\alpha'} = 0$, choose $(\hat{f}'_j)_{j=1,2,3}$ to be any RHON basis with $\hat{f}'_1 = \hat{b}'$.

Use the previous paragraph with all primes removed to define α and $(\hat{f}_j)_{j=1,2,3}$.

QED

Suppose we are given a matrix which is known to be the LO-RHS invariant $\mathcal{G}_2^{(2)}$ of a quantum circuit with 2-qubits and 2 DC-NOTs. Furthermore, we are asked to extract from this matrix values (non-unique ones) for $\hat{a}, \hat{b}, \hat{a}'$ and \hat{b}' . Next we will give an algorithm for accomplishing this task. We will call it our “Algorithm for Diagonalizing $\mathcal{G}_2^{(2)}$ ”. The algorithm first expresses $\mathcal{G}_2^{(2)}$ in term of its principal parameters. Then it solves for $\hat{a}, \hat{b}, \hat{a}'$ and \hat{b}' in terms of these parameters.

Algorithm for Diagonalizing $\mathcal{G}_2^{(2)}$:

1. Set $\lambda_{2r} = \frac{1}{4}\text{tr}(\mathcal{G}_2^{(2)})$. Set $\Delta = \mathcal{G}_2^{(2)} - \lambda_{2r}$, $\Lambda_{2r} = (\Delta + \Delta^\dagger)/2$ and $\Lambda_{2i} = (\Delta - \Delta^\dagger)/(2i)$. Hence, $\mathcal{G}_2^{(2)} = \lambda_{2r} + \Lambda_{2r} + i\Lambda_{2i}$, where λ_{2r} is a real scalar, and $\Lambda_{2r}, \Lambda_{2i}$ are traceless Hermitian matrices.
2. Calculate $c_{\alpha'}c_\alpha$, $s_{\alpha'}s_\alpha$, \hat{f}_2 and \hat{f}'_2 from Λ_{2r} and Λ_{2i} . (If $\Lambda_{2r} = 0$, then take $s_{\alpha'}s_\alpha = 0$, and choose \hat{f}_2 and \hat{f}'_2 to be any 3d unit vectors.)
3. Choose any RHON basis $(\hat{h}_j)_{j=1,2,3}$ such that $\hat{h}_2 = \hat{f}_2$, and any RHON basis $(\hat{h}'_j)_{j=1,2,3}$ such that $\hat{h}'_2 = \hat{f}'_2$.
4. Find a Singular Value Decomposition (SVD) of the matrix

$$M = \begin{bmatrix} \hat{h}_3'^T \Lambda_{2i} \hat{h}_1 & \hat{h}_3'^T \Lambda_{2i} \hat{h}_3 \\ \hat{h}_1'^T \Lambda_{2i} \hat{h}_1 & \hat{h}_1'^T \Lambda_{2i} \hat{h}_3 \end{bmatrix} . \quad (92)$$

In other words, find 2-dimensional orthogonal matrices U, V and a non-negative 2-dimensional diagonal matrix D such that

$$M = UDV^T . \quad (93)$$

Now calculate $s_{\alpha'}c_\alpha$, $c_{\alpha'}s_\alpha$, \hat{f}'_3 , \hat{f}'_1 , \hat{f}_3 , \hat{f}_1 from

$$\begin{bmatrix} s_{\alpha'}c_\alpha & 0 \\ 0 & c_{\alpha'}s_\alpha \end{bmatrix} = D , \quad (94)$$

$$[\hat{f}'_3, \hat{f}'_1] = [\hat{h}'_3, \hat{h}'_1]U , \quad (95)$$

and

$$[\hat{f}_1, \hat{f}_3] = [\hat{h}_1, \hat{h}_3]V . \quad (96)$$

5. By expressing U on the RHS of Eq.(95) in component form, it is easy to verify that

$$\hat{f}'_3 \times \hat{f}'_1 = \det(U) \hat{h}'_3 \times \hat{h}'_1 . \quad (97)$$

$\hat{h}'_3 \times \hat{h}'_1 \cdot \hat{h}'_2 = +1$ and $\hat{f}'_2 = \hat{h}'_2$ so

$$\hat{f}'_3 \times \hat{f}'_1 \cdot \hat{f}'_2 = \det(U) . \quad (98)$$

$\det(U)$ will always equal either $+1$ or -1 . If $\det(U) = -1$, replace $\hat{f}'_3 \rightarrow -\hat{f}'_3$ and $s_{\alpha'}c_{\alpha} \rightarrow -s_{\alpha'}c_{\alpha}$. These replacements make $(\hat{f}'_1, \hat{f}'_2, \hat{f}'_3)$ a right handed basis. If $\det(V) = -1$, an analogous procedure can be used to convert $(\hat{f}_1, \hat{f}_2, \hat{f}_3)$ into a right-handed basis.

6. At this point, we know the four quantities $c_{\alpha'}c_{\alpha}$, $s_{\alpha'}c_{\alpha}$, $c_{\alpha'}s_{\alpha}$, and $s_{\alpha'}s_{\alpha}$. Calculate $\alpha' \pm \alpha$ from

$$\cos(\alpha' \pm \alpha) = c_{\alpha'}c_{\alpha} \mp s_{\alpha'}s_{\alpha} , \quad (99a)$$

and

$$\sin(\alpha' \pm \alpha) = s_{\alpha'}c_{\alpha} \pm c_{\alpha'}s_{\alpha} . \quad (99b)$$

Calculate (α', α) from $\alpha' \pm \alpha$.

7. Calculate $\hat{a}, \hat{b}, \hat{a}', \hat{b}'$ from:

$$\begin{cases} \hat{b} = \hat{f}_1 \\ \hat{a} = c_{\alpha}\hat{f}_1 - s_{\alpha}\hat{f}_2 \end{cases} , \quad \begin{cases} \hat{b}' = \hat{f}'_1 \\ \hat{a}' = c_{\alpha'}\hat{f}'_1 - s_{\alpha'}\hat{f}'_2 \end{cases} . \quad (100)$$

8.3 Invariant for Circuits with 3 DC-NOTs

[`ckt_invar123.m`, `ckt_invar3.m`, `diag_ckt_invar3.m`, `test_diag_invar3.m`]

This part of our program is dedicated to the letters $\mathcal{G}_3^{(2)}$.

Theorem 19

$$\mathcal{G}_3^{(2)} = \begin{array}{c} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} -\hat{a} \text{---} -\hat{b} \text{---} -\hat{c} \text{---} \\ | \quad | \quad | \quad | \quad | \quad | \\ \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} -\hat{a}' \text{---} -\hat{b}' \text{---} -\hat{c}' \text{---} \end{array} \quad (101a)$$

$$= \lambda_{3r} + i\lambda_{3i} + \Lambda_{3r} + i\Lambda_{3i}, \quad (101b)$$

where

$$\lambda_{3r} = [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' \quad [\hat{a}\hat{b}\hat{b}] \cdot \hat{c}, \quad (102)$$

$$\lambda_{3i} = -(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})\mathcal{V}' - (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\mathcal{V}, \quad (103)$$

$$\Lambda_{3r} = \begin{cases} -(\hat{a}' \cdot \hat{b}')(\hat{a} \cdot \hat{b})\sigma_{\hat{c}',\hat{c}} \\ +(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})\sigma_{[\hat{a}'\hat{b}'\hat{c}'],\hat{c}} + (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\sigma_{\hat{c}',[\hat{a}\hat{b}\hat{c}]} \\ +(\hat{a}' \cdot \hat{b}')\mathcal{V}\sigma_{[\hat{b}'\hat{c}'],\hat{c}} + (\hat{a} \cdot \hat{b})\mathcal{V}'\sigma_{\hat{c}',[\hat{b}\hat{c}]} \\ -\sigma_{[\hat{a}'\hat{b}'\hat{b}'\hat{c}'\hat{c}'],[\hat{a}\hat{b}\hat{b}\hat{c}\hat{c}]} \end{cases}, \quad (104)$$

$$\Lambda_{3i} = \begin{cases} +(\hat{a} \cdot \hat{b})\sigma_{[\hat{a}'\hat{b}'\hat{c}'\hat{c}'],[\hat{b}\hat{c}\hat{c}]} + (\hat{a}' \cdot \hat{b}')\sigma_{[\hat{b}'\hat{c}'\hat{c}'],[\hat{a}\hat{b}\hat{c}\hat{c}]} \\ +[\hat{a}\hat{b}\hat{b}] \cdot \hat{c}\sigma_{[\hat{a}'\hat{b}'\hat{b}'\hat{c}'],\hat{c}} + [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}'\sigma_{\hat{c}',[\hat{a}\hat{b}\hat{b}\hat{c}]} \end{cases}, \quad (105)$$

where $\mathcal{V} = \hat{a} \times \hat{b} \cdot \hat{c}$ and $\mathcal{V}' = \hat{a}' \times \hat{b}' \cdot \hat{c}'$.

proof:

$$\mathcal{G}_3^{(2)} = \begin{array}{c} \text{---} \hat{c} \text{---} \\ | \\ \text{---} \hat{c}' \text{---} \end{array} \mathcal{G}_2^{(2)} \begin{array}{c} \text{---} -\hat{c} \text{---} \\ | \\ \text{---} -\hat{c}' \text{---} \end{array} \quad (106a)$$

$$= \begin{array}{c} \text{---} \hat{c} \text{---} \\ | \\ \text{---} \hat{c}' \text{---} \end{array} \mathcal{G}_2^{(2)} \begin{array}{c} \text{---} \hat{c} \text{---} \\ | \\ \text{---} \hat{c}' \text{---} \end{array} (-\sigma_{\hat{c}',\hat{c}}). \quad (106b)$$

An explicit expression for $\mathcal{G}_2^{(2)}$ was given in Section 8.2. Eq.(27) shows how to calculate the effect of DC-NOT similarity transformations.

QED

Theorem 20 Suppose

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \\ \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{c}_f \text{---} \hat{b}_f \text{---} \hat{a}_f \text{---} \\ | \quad | \quad | \\ \text{---} \hat{c}'_f \text{---} \hat{b}'_f \text{---} \hat{a}'_f \text{---} \end{array}. \quad (107)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$, and such that (a) $\hat{a}_f \times \hat{b}_f \cdot \hat{c}_f = 0$, and (b) $\hat{b}'_f \perp \text{span}(\hat{c}'_f, \hat{a}'_f)$.

proof:

As pointed out in the introduction, Ref.[6] shows how to express any 2-qubit unitary operation as a circuit with just 3-CNOTs. It is easy to check that conditions (a) and (b) are satisfied by the 3-CNOT circuit given in Ref.[6]. Hence, this theorem has already been proven in Ref.[6], although Ref.[6] does not explicitly point out this property of their 3-CNOT circuit. The “Algorithm for Diagonalizing $\mathcal{G}_3^{(2)}$ ”, that is presented later in this section, also constitutes a (constructive) proof of this theorem.

QED

For $A, B \in \mathbb{R}^{p \times q}$, define the following two commutators:

$$[A, B]_L = A^T B - B^T A , \quad (108a)$$

$$[A, B]_R = AB^T - BA^T . \quad (108b)$$

(Here, the letters L and R stand for left and right. They indicate on which matrix the transpose symbol acts, either the left or the right matrix in the matrix product.) Ref.[7] presents a proof (due to Eckart and Young) of the following Theorem. $A, B \in \mathbb{R}^{p \times q}$ have a simultaneous Singular Value Decomposition (SVD) if and only if $[A, B]_L$ and $[A, B]_R$ are both zero. By a simultaneous SVD we mean orthogonal matrices U, V and real diagonal matrices D_A, D_B such that

$$A = UD_A V^T , \quad B = UD_B V^T . \quad (109)$$

When considering the SVD of a single matrix A , one usually insists in making the entries of D_A non-negative, and calling them the singular values of A . In the case of a simultaneous SVD, one can't always make both diagonal matrices non-negative, but one can certainly make one of them so.

Of course, the previous paragraph applies almost intact if A and B are elements of $\mathbb{C}^{p \times q}$ instead of $\mathbb{R}^{p \times q}$. For A, B complex, one must replace the T (transpose) symbol by the \dagger (Hermitian conjugate) symbol in Eqs.(108) and (109). Also, the matrices U, V in Eq.(109) must be unitary instead of orthogonal.

Note that when A and B are Hermitian, the condition that $[A, B]_L$ and $[A, B]_R$ both vanish becomes simply the condition that A and B commute. The Eckart, Young theorem then becomes a theorem very familiar to practitioners of Quantum Mechanics: two Hermitian operators can be simultaneously diagonalized iff they commute.

Theorem 21

$$[\Lambda_{3r}, \Lambda_{3i}] = 0 , \quad (110)$$

$$[\Lambda_{3r}^\Gamma, \Lambda_{3i}^\Gamma]_L = 0 , \quad (111)$$

$$[\Lambda_{3r}^\Gamma, \Lambda_{3i}^\Gamma]_R = 0 . \quad (112)$$

proof:

Let

$$\Delta = \mathcal{G}_3^{(2)} - \text{tr}(\mathcal{G}_3^{(2)}) , \quad (113)$$

so

$$\Lambda_{3r} = \frac{\Delta + \Delta^\dagger}{2} , \quad \Lambda_{3i} = \frac{\Delta - \Delta^\dagger}{2i} . \quad (114)$$

Thus,

$$[\Lambda_{3r}, \Lambda_{3i}] = \frac{1}{4i}[\Delta + \Delta^\dagger, \Delta - \Delta^\dagger] = \frac{1}{2i}[\Delta^\dagger, \Delta] = \frac{1}{2i}[\mathcal{G}_3^{(2)\dagger}, \mathcal{G}_3^{(2)}] = 0 , \quad (115)$$

where the last commutator is zero because $\mathcal{G}_3^{(2)}$ is unitary.

Note that for any $\hat{a}, \hat{a}', \hat{b}, \hat{b}' \in \mathbb{R}^3$,

$$[\sigma_{\hat{a}', \hat{a}}, \sigma_{\hat{b}', \hat{b}}] = \begin{cases} +(\hat{a}' \cdot \hat{b}' + i\sigma_{\hat{a}' \times \hat{b}'}) \otimes (\hat{a} \cdot \hat{b} + i\sigma_{\hat{a} \times \hat{b}}) \\ -(\hat{b}' \cdot \hat{a}' + i\sigma_{\hat{b}' \times \hat{a}'}) \otimes (\hat{b} \cdot \hat{a} + i\sigma_{\hat{b} \times \hat{a}}) \end{cases} \quad (116a)$$

$$= i2[(\hat{a} \cdot \hat{b})\sigma_{\hat{a}' \times \hat{b}', 1} - (\hat{a}' \cdot \hat{b}')\sigma_{1, \hat{a} \times \hat{b}}] . \quad (116b)$$

From Theorem 19, we know that Λ_{3r} and Λ_{3i} can be expressed in the form

$$\Lambda_{3r} = \sum_j \alpha_j \sigma_{\hat{a}'_j, \hat{a}_j} , \quad \Lambda_{3i} = \sum_k \beta_k \sigma_{\hat{b}'_k, \hat{b}_k} , \quad (117)$$

for some $\alpha_j, \beta_j \in \mathbb{R}$ and $\hat{a}_j, \hat{a}'_j, \hat{b}_k, \hat{b}'_k \in \mathbb{R}^3$. Therefore,

$$0 = [\Lambda_{3r}, \Lambda_{3i}] \quad (118a)$$

$$= \sum_{j,k} \alpha_j \beta_k [\sigma_{\hat{a}'_j, \hat{a}_j}, \sigma_{\hat{b}'_k, \hat{b}_k}] \quad (118b)$$

$$= i2 \sum_{j,k} \alpha_j \beta_k [(\hat{a}_j \cdot \hat{b}_k)\sigma_{\hat{a}'_j \times \hat{b}'_k, 1} - (\hat{a}'_j \cdot \hat{b}'_k)\sigma_{1, \hat{a}_j \times \hat{b}_k}] . \quad (118c)$$

This implies that

$$\sum_{j,k} \alpha_j \beta_k (\hat{a}_j \cdot \hat{b}_k) \hat{a}'_j \times \hat{b}'_k = 0 , \quad \sum_{j,k} \alpha_j \beta_k (\hat{a}'_j \cdot \hat{b}'_k) \hat{a}_j \times \hat{b}_k = 0 . \quad (119)$$

Now note that

$$[\Lambda_{3r}^\Gamma, \Lambda_{3i}^\Gamma]_R = \left(\sum_j \alpha_j \hat{a}'_j \hat{a}_j^T \right) \left(\sum_k \beta_k \hat{b}_k \hat{b}_k'^T \right) - \left(\sum_k \beta_k \hat{b}'_k \hat{b}_k^T \right) \left(\sum_j \alpha_j \hat{a}_j \hat{a}_j'^T \right) \quad (120a)$$

$$= \sum_{j,k} \alpha_j \beta_k (\hat{a}_j^T \hat{b}_k) [\hat{a}'_j \hat{b}_k'^T - \hat{b}'_k \hat{a}_j'^T] \quad (120b)$$

$$= 0 , \quad (120c)$$

where the last expression vanishes due to Eq.(119). An analogous argument shows that $[\Lambda_{3r}^\Gamma, \Lambda_{3i}^\Gamma]_L$ also vanishes.

QED

It is convenient to parameterize the expression for $\mathcal{G}_3^{(2)}$ given by Theorem 19, using as few parameters as possible.

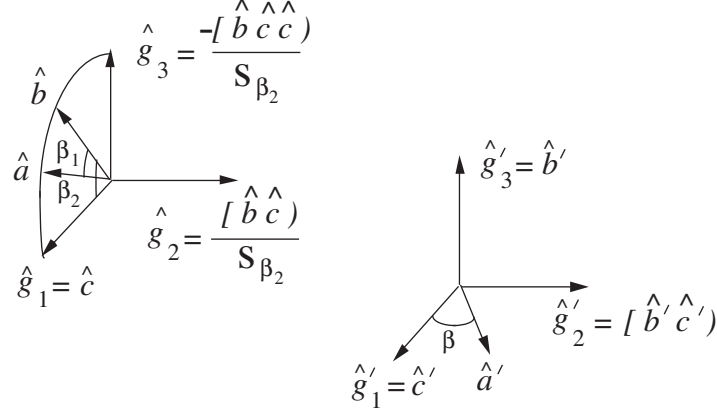


Figure 8: Principal parameters of $\mathcal{G}_3^{(2)}$.

Theorem 22 $\mathcal{G}_3^{(2)}$ can be parameterized with 3 real numbers β, β_1, β_2 , and 2 RHON bases $(\hat{g}_j)_{j=1,2,3}$ and $(\hat{g}'_j)_{j=1,2,3}$. Call these the principal parameters of $\mathcal{G}_3^{(2)}$ (see Fig.8). More explicitly,

$$\mathcal{G}_3^{(2)} = \lambda_{3r} + i\lambda_{3i} + \Lambda_{3r} + i\Lambda_{3i} , \quad (121)$$

where

$$\lambda_{3r} = -X_o , \quad (122)$$

$$\lambda_{3i} = -Y_o , \quad (123)$$

$$\Lambda_{3r} = \sum_{j=1}^3 \nu_j \hat{g}'_j \hat{g}_{\pi(j)}^T , \quad (124)$$

$$\Lambda_{3i} = \sum_{j=1}^3 \mu_j \hat{g}'_j \hat{g}_{\pi(j)}^T , \quad (125)$$

where

$$X_o = c_\beta \xi s_{\beta_1} s_{\beta_2} , \quad (126)$$

$$Y_o = s_\beta c_{\beta_1} c_{\beta_2} , \quad (127)$$

$$(\nu_j)_{j=1,2,3} = (s_\beta c_{\beta_1} s_{\beta_2}, s_\beta s_{\beta_1} |c_{\beta_2}|, c_\beta c_{\beta_1} c_{\beta_2}) , \quad (128)$$

$$(\mu_j)_{j=1,2,3} = (-c_\beta s_{\beta_1} |c_{\beta_2}|, -c_\beta c_{\beta_1} s_{\beta_2}, s_\beta \xi s_{\beta_1} s_{\beta_2}) , \quad (129)$$

where $\xi \in \{+1, -1\}$ and $\pi()$ is the permutation $\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$.

proof:

We will assume from the onset of this proof that (a) $\hat{a} \times \hat{b} \cdot \hat{c} = 0$, and (b) $\hat{b}' \perp \text{span}(\hat{c}', \hat{a}')$. This can be assumed without loss of generality because of Theorem 20.

Let

$$\xi = \text{sign}([ab] \cdot [bc]) , \quad \xi_2 = \text{sign}(\hat{b} \cdot \hat{c}) . \quad (130)$$

Without loss of generality, we will assume that $-\xi\xi_2 = +1$. If $-\xi\xi_2$ is initially negative, we can make it positive by replacing both \hat{a} and \hat{a}' by their negatives. This replacement will not change $\mathcal{G}_3^{(2)}$. Using the circuit shown in Eq.(101a), it is easy to prove that $\mathcal{G}_3^{(2)}$ is odd in both \hat{a} and \hat{a}' .

Define

$$s_{\beta_2} = |[\hat{b}\hat{c}]| , \quad \eta = |[\hat{a}\hat{b}\hat{b}\hat{c}]| = |[\hat{a}\hat{b}]\hat{b} \cdot \hat{c}| . \quad (131)$$

To begin, we will assume that $s_{\beta_2} \neq 0$ and $\eta \neq 0$. Later on, before ending the proof, we will remove these two constraints.

If we define

$$X_o = (\hat{a}' \cdot \hat{c}') [\hat{a}\hat{b}\hat{b}] \cdot \hat{c} , \quad (132)$$

$$Y_o = (\hat{a} \cdot \hat{b}) (\hat{b} \cdot \hat{c}) \mathcal{V}' , \quad (133)$$

$$(\hat{g}'_j)_{j=1,2,3} = (\hat{c}', [\hat{b}'\hat{c}'], \hat{b}') , \quad (134)$$

$$(\hat{g}_j)_{j=1,2,3} = (\hat{c}, \frac{[\hat{b}\hat{c}]}{s_{\beta_2}}, \frac{-[\hat{b}\hat{c}\hat{c}]}{s_{\beta_2}}) , \quad (135)$$

$$(\nu_j)_{j=1,2,3} = \left(\hat{a} \cdot \hat{b} \mathcal{V}' s_{\beta_2}, \mathcal{V}' \eta, (\hat{a} \cdot \hat{b}) (\hat{b} \cdot \hat{c}) (\hat{a}' \cdot \hat{c}') \right) , \quad (136a)$$

$$(\hat{v}_j)_{j=1,2,3} = \left(\frac{[\hat{b}\hat{c}]}{s_{\beta_2}}, \frac{-[\hat{a}\hat{b}\hat{b}\hat{c}\hat{c}]}{\eta}, \hat{c} \right) , \quad (136b)$$

$$(\mu_j)_{j=1,2,3} = \left(-\hat{a}' \cdot \hat{c}' \eta, -(\hat{a} \cdot \hat{b}) (\hat{a}' \cdot \hat{c}') s_{\beta_2}, [\hat{a}\hat{b}\hat{b}] \cdot \hat{c} \mathcal{V}' \right) , \quad (137a)$$

$$(\hat{u}_j)_{j=1,2,3} = \left(\frac{[\hat{a}\hat{b}\hat{b}\hat{c}]}{\eta}, \frac{-[\hat{b}\hat{c}\hat{c}]}{s_{\beta_2}}, \hat{c} \right), \quad (137b)$$

then

$$\mathcal{G}_3^{(2)} = -X_o - iY_o + \sum_{j=1}^3 \nu_j \hat{g}'_j \hat{v}_j^T + i \sum_{j=1}^3 \mu_j \hat{g}'_j \hat{u}_j^T. \quad (138)$$

Define an angle β by

$$\cos(\beta) = \hat{a}' \cdot \hat{c}', \quad \sin(\beta) = \mathcal{V}'. \quad (139)$$

Define angles $\beta_1, \beta_2 \in [0, \pi)$ by

$$\cos(\beta_1) = \hat{a} \cdot \hat{b}, \quad \sin(\beta_1) = |\hat{a} \times \hat{b}|, \quad (140)$$

and

$$\cos(\beta_2) = \hat{b} \cdot \hat{c}, \quad \sin(\beta_2) = |\hat{b} \times \hat{c}|. \quad (141)$$

Hence, $[\hat{a}\hat{b}]/s_{\beta_1} = \xi[\hat{b}\hat{c}]/s_{\beta_2}$. One finds

$$\eta = s_{\beta_1} |c_{\beta_2}|, \quad (142)$$

$$\frac{[\hat{a}\hat{b}\hat{b}\hat{c}]}{\eta} \cdot \hat{g}_2 = -\xi \xi_2, \quad (143)$$

$$\frac{-[\hat{a}\hat{b}\hat{b}\hat{c}\hat{c}]}{\eta} \cdot \hat{g}_3 = -\xi \xi_2, \quad (144)$$

and

$$[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = \xi s_{\beta_1} s_{\beta_2}. \quad (145)$$

At this point, it is easy re-express various quantities in terms of the principal parameters. Eq.(132) for X_o , Eq.(133) for Y_o , Eq.(136a) for the ν_j , and Eq.(137a) for the μ_j , yield, respectively, Eq.(126), Eq.(127), Eq.(128), and Eq.(129).

We can also re-express Eqs.(136b) and (137b) for the \hat{v}_j and \hat{u}_j in terms of the principal parameters. One finds

$$(\hat{v}_j)_{j=1,2,3} = (\hat{g}_2, -\xi \xi_2 \hat{g}_3, \hat{g}_1) = (\hat{g}_2, \hat{g}_3, \hat{g}_1), \quad (146)$$

and

$$(\hat{u}_j)_{j=1,2,3} = (-\xi \xi_2 \hat{g}_2, \hat{g}_3, \hat{g}_1) = (\hat{g}_2, \hat{g}_3, \hat{g}_1). \quad (147)$$

Hence, for $j = 1, 2, 3$,

$$\hat{v}_j = \hat{u}_j = \hat{g}_{\pi(j)} . \quad (148)$$

When s_{β_2} or η vanish, Eq.(135) fails to define two of the vectors \hat{g}_j , Eq.(136b) fails to define one or two of the vectors \hat{v}_j , and Eq.(137b) fails to define one or two of the vectors \hat{u}_j . If $s_{\beta_2} = 0$, the proof survives if we define $(\hat{g}_j)_{j=1,2,3}$ to be any RHON basis such that $\hat{g}_1 = \hat{c}$ and $\hat{g}_2 \perp \text{span}(\hat{a}, \hat{b}, \hat{c})$. Then define the \hat{u}_j and \hat{v}_j vectors in accordance with Eq.(148). If $\eta = 0$ but $s_{\beta_2} \neq 0$, define the \hat{u}_j and \hat{v}_j vectors in accordance with Eq.(148).

QED

Suppose we are given a matrix which is known to be the LO-RHS invariant $\mathcal{G}_3^{(2)}$ of a quantum circuit with 2-qubits and 3 DC-NOTs. Furthermore, we are asked to extract from this matrix values (non-unique ones) for \hat{a} , \hat{b} , \hat{c} , \hat{a}' , \hat{b}' and \hat{c}' . Next we will give an algorithm for accomplishing this task. We will call it our “Algorithm for Diagonalizing $\mathcal{G}_3^{(2)}$ ”. The algorithm first expresses $\mathcal{G}_3^{(2)}$ in term of its principal parameters. Then it solves for \hat{a} , \hat{b} , \hat{c} , \hat{a}' , \hat{b}' and \hat{c}' in terms of these parameters.

Algorithm for Diagonalizing $\mathcal{G}_3^{(2)}$:

1. Set $\lambda_{3r} = \frac{1}{4}\text{Re}[\text{tr}(\mathcal{G}_3^{(2)})]$ and $\lambda_{3i} = \frac{1}{4}\text{Im}[\text{tr}(\mathcal{G}_3^{(2)})]$. Set $\Delta = \mathcal{G}_3^{(2)} - \text{tr}(\mathcal{G}_3^{(2)})$, $\Lambda_{3r} = (\Delta + \Delta^\dagger)/2$ and $\Lambda_{3i} = (\Delta - \Delta^\dagger)/(2i)$. Hence, $\mathcal{G}_3^{(2)} = \lambda_{3r} + i\lambda_{3i} + \Lambda_{3r} + i\Lambda_{3i}$, where $\lambda_{3r}, \lambda_{3i}$ are real scalars, and $\Lambda_{3r}, \Lambda_{3i}$ are traceless Hermitian matrices.
2. Set $X_o = -\lambda_{3r}$ and $Y_o = -\lambda_{3i}$.
3. Do a simultaneous SVD of Λ_{3r}^Γ and Λ_{3i}^Γ . This decomposition is possible since we have shown previously that $[\Lambda_{3r}^\Gamma, \Lambda_{3i}^\Gamma]_L$ and $[\Lambda_{3r}^\Gamma, \Lambda_{3i}^\Gamma]_R$ are both zero. The decomposition yields orthogonal matrices U, V and real diagonal matrices D_{3r}, D_{3i} such that

$$\Lambda_{3r}^\Gamma = U D_{3r} V^T , \quad \Lambda_{3i}^\Gamma = U D_{3i} V^T . \quad (149)$$

For $j = 1, 2, 3$, set

$$\nu_j = (D_{3r})_{jj} , \quad \mu_j = (D_{3i})_{jj} . \quad (150)$$

Set

$$[\hat{g}'_1, \hat{g}'_2, \hat{g}'_3] = U , \quad [\hat{g}_1, \hat{g}_2, \hat{g}_3] = V . \quad (151)$$

4. Set $\xi = \text{sign}(\mu_3 \nu_2)$. Set $\xi_2 = -\xi$. Calculate β from

$$c_\beta = \xi \frac{X_o}{\sqrt{\mu_3^2 + X_o^2}} , \quad s_\beta = \xi \frac{\mu_3}{\sqrt{\mu_3^2 + X_o^2}} . \quad (152)$$

If $|c_\beta| \geq |s_\beta|$, set

$$\begin{bmatrix} c_{\beta_1} c_{\beta_2} & c_{\beta_1} s_{\beta_2} \\ s_{\beta_1} c_{\beta_2} & s_{\beta_1} s_{\beta_2} \end{bmatrix} = \frac{1}{c_\beta} \begin{bmatrix} \nu_3 & -\mu_2 \\ -\xi_2 \mu_1 & \xi X_o \end{bmatrix}. \quad (153)$$

On the other hand, if $|s_\beta| \geq |c_\beta|$, set

$$\begin{bmatrix} c_{\beta_1} c_{\beta_2} & c_{\beta_1} s_{\beta_2} \\ s_{\beta_1} c_{\beta_2} & s_{\beta_1} s_{\beta_2} \end{bmatrix} = \frac{1}{s_\beta} \begin{bmatrix} Y_o & \nu_1 \\ \xi_2 \nu_2 & \xi \mu_3 \end{bmatrix}. \quad (154)$$

5. At this point, we know the four quantities $c_{\beta_1} c_{\beta_2}$, $s_{\beta_1} c_{\beta_2}$, $c_{\beta_1} s_{\beta_2}$, and $s_{\beta_1} s_{\beta_2}$. Calculate $\beta_1 \pm \beta_2$ from

$$\cos(\beta_1 \pm \beta_2) = c_{\beta_1} c_{\beta_2} \mp s_{\beta_1} s_{\beta_2}, \quad (155a)$$

and

$$\sin(\beta_1 \pm \beta_2) = s_{\beta_1} c_{\beta_2} \pm c_{\beta_1} s_{\beta_2}. \quad (155b)$$

Calculate (β_1, β_2) from $\beta_1 \pm \beta_2$.

6. At this point, $s_{\beta_1} s_{\beta_2}$ is guaranteed to be positive, but there is not guarantee that s_{β_1} and s_{β_2} are individually positive (they may both be negative). Furthermore, at this point there is no guarantee that $\xi_2 = \text{sign}(c_{\beta_2})$. These disagreements with the assumptions of our parameterization can be fixed as follows. If $s_{\beta_1} < 0$, replace β_1 and β_2 by their negatives, and replace $(\hat{g}'_1, \hat{g}'_2, \nu_1, \nu_2, \mu_1, \mu_2)$ each by its negative. If $\xi_2 c_{\beta_2} < 0$, replace $\beta_1 \rightarrow \pi - \beta_1$ and $\beta_2 \rightarrow \pi - \beta_2$, and replace $(\hat{g}'_1, \hat{g}'_2, \nu_1, \nu_2, \mu_1, \mu_2)$ each by its negative.

7. Calculate $\hat{a}, \hat{b}, \hat{c}, \hat{a}', \hat{b}', \hat{c}'$ from:

$$\begin{cases} \hat{c} = \hat{g}_1 \\ \hat{b} = c_{\beta_2} \hat{g}_1 + s_{\beta_2} \hat{g}_3 \\ \hat{a} = \cos(\beta_2 - \xi_2 \beta_1) \hat{g}_1 + \sin(\beta_2 - \xi_2 \beta_1) \hat{g}_3 \end{cases}, \quad \begin{cases} \hat{c}' = \hat{g}'_1 \\ \hat{b}' = \hat{g}'_3 \\ \hat{a}' = c_\beta \hat{g}'_1 + s_\beta \hat{g}'_2 \end{cases}. \quad (156)$$

Note the ξ_2 's in the expression for \hat{a} . The reason for these ξ_2 's is that in order to obey $-\xi \xi_2 = +1$, one must define the sign of the angle β_1 differently depending on whether c_{β_2} is positive or negative. (See Fig.9)

Theorem 23 For any $j \in \{1, 2, 3\}$,

$$\mu_j \nu_j = X_o Y_o. \quad (157)$$

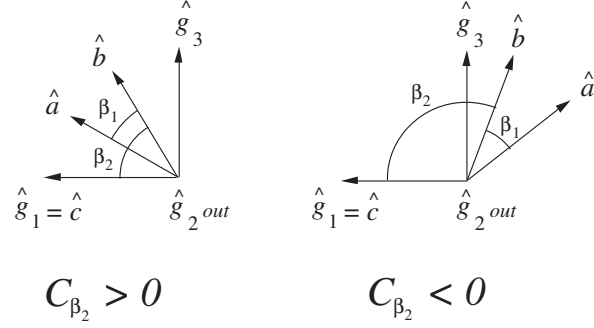


Figure 9: Sign of β_1 is defined differently depending on whether c_{β_2} is positive or negative.

If i, j, k are 3 distinct element of $\{1, 2, 3\}$, then

$$\mu_i \mu_j = -X_o \nu_k, \quad (158)$$

and

$$\nu_i \nu_j = -Y_o \mu_k. \quad (159)$$

proof:

Follows from the definitions Eq.(126) for X_o , Eq.(127) for Y_o , Eq.(128) for the ν_j , and Eq.(129) for the μ_j .

QED

Define Π to be the permutation matrix that corresponds to the permutation map $\pi()$ used above. Thus,

$$\Pi = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}. \quad (160)$$

If $(s_j)_{j=1,2,3}$ denotes the standard basis, define matrices M_μ and M_ν by

$$M_\mu = \sum_{j=1}^3 \mu_j \hat{s}_j \hat{s}_{\pi(j)} \quad (161a)$$

$$= \text{diag}(\mu_1, \mu_2, \mu_3) \Pi, \quad (161b)$$

and

$$M_\nu = \sum_{j=1}^3 \nu_j \hat{s}_j \hat{s}_{\pi(j)} \quad (162a)$$

$$= \text{diag}(\nu_1, \nu_2, \nu_3) \Pi. \quad (162b)$$

Note that Λ_{2r}^Γ (given by Eq.(124)) becomes M_ν and Λ_{2i}^Γ (given by Eq.(125)) becomes M_μ when the bases $(\hat{g}_j)_{j=1,2,3}$ and $(\hat{g}'_j)_{j=1,2,3}$ are both rotated into the standard basis.

Theorem 24

$$M_\mu M_\nu^T = M_\nu M_\mu^T = X_o Y_o , \quad (163)$$

$$M_\mu^T M_\nu = M_\nu^T M_\mu = X_o Y_o , \quad (164)$$

and

$$(M_\mu^T)^2 = \text{tr}(M_\nu) - M_\nu . \quad (165)$$

proof:

Follows from Theorem 23.

QED

8.4 Invariant for Circuits with 4 DC-NOTs

[ckt_invar4.m]

This part of our program is dedicated to the letters $\mathcal{G}_4^{(2)}$.

Theorem 25

$$\mathcal{G}_4^{(2)} = \begin{array}{cccccccc} \textcircled{\hat{d}} & \textcircled{\hat{c}} & \textcircled{\hat{b}} & \textcircled{\hat{a}} & \textcircled{-\hat{a}} & \textcircled{-\hat{b}} & \textcircled{-\hat{c}} & \textcircled{-\hat{d}} \\ | & | & | & | & | & | & | & | \\ \textcircled{\hat{d}'} & \textcircled{\hat{c}'} & \textcircled{\hat{b}'} & \textcircled{\hat{a}'} & \textcircled{-\hat{a}'} & \textcircled{-\hat{b}'} & \textcircled{-\hat{c}'} & \textcircled{-\hat{d}'} \end{array} \quad (166a)$$

$$= \lambda_{4r} + i\lambda_{4i} + \Lambda_{4r} + i\Lambda_{4i} , \quad (166b)$$

where

$$\lambda_{4r} = - \sum_j (\hat{g}'_j \cdot \hat{d}') \nu_j \hat{g}_{\pi(j)} \cdot \hat{d} , \quad \lambda_{4i} = (\lambda_{4r})_{\nu \rightarrow \mu} , \quad (167)$$

$$\Lambda_{4r} = X_o \sigma_{\hat{d}', \hat{d}} + \sigma_{\vec{x}', \hat{d}} + \sigma_{\hat{d}', \vec{x}} + \Delta X , \quad (168)$$

$$\Lambda_{4i} = Y_o \sigma_{\hat{d}', \hat{d}} - \sigma_{\vec{y}', \hat{d}} - \sigma_{\hat{d}', \vec{y}} + \Delta Y , \quad (169)$$

where

$$\vec{x} = \sum_j \mu_j (\hat{g}'_j \cdot \hat{d}') [\hat{g}_{\pi(j)} \hat{d}] , \quad \vec{y} = (\vec{x})_{\mu \rightarrow \nu} , \quad (170)$$

$$\vec{x}' = \sum_j \mu_j (\hat{g}_{\pi(j)} \cdot \hat{d}) [\hat{g}'_j \hat{d}'] , \quad \vec{y}' = (\vec{x}')_{\mu \rightarrow \nu} , \quad (171)$$

$$\Delta X = \sum_j \nu_j \sigma_{[\hat{g}'_j \hat{d}' \hat{d}'], [\hat{g}_{\pi(j)} \hat{d} \hat{d}]} , \quad \Delta Y = (\Delta X)_{\nu \rightarrow \mu} , \quad (172)$$

where any variables not already defined in the statement of this theorem are defined in Section 8.3.

proof:

$$\mathcal{G}_4^{(2)} = \begin{array}{c} \text{---} \hat{d} \text{---} \\ | \\ \text{---} \hat{d}' \text{---} \end{array} \mathcal{G}_3^{(2)} = \begin{array}{c} \text{---} -\hat{d} \text{---} \\ | \\ \text{---} -\hat{d}' \text{---} \end{array} \quad (173a)$$

$$= \begin{array}{c} \text{---} \hat{d} \text{---} \\ | \\ \text{---} \hat{d}' \text{---} \end{array} \mathcal{G}_3^{(2)} \begin{array}{c} \text{---} \hat{d} \text{---} \\ | \\ \text{---} \hat{d}' \text{---} \end{array} (-\sigma_{\hat{d}', \hat{d}}) . \quad (173b)$$

An explicit expression for $\mathcal{G}_3^{(2)}$ was given in Section 8.3. Eq.(27) shows how to calculate the effect of DC-NOT similarity transformations.

QED

Theorem 26 When the bases $(\hat{g}_j)_{j=1,2,3}$ and $(\hat{g}'_j)_{j=1,2,3}$ are both taken to be the standard basis, then the quantities λ_{4r} , λ_{4i} , \vec{x} , \vec{y} , \vec{x}' , \vec{y}' , ΔX and ΔY (all defined in Theorem 25) can be expressed in terms of the matrices M_μ, M_ν and the vectors \hat{d}, \hat{d}' as follows:

$$\lambda_{4r} = -\hat{d}'^T M_\nu \hat{d} , \quad \lambda_{4i} = (\lambda_{4r})_{\nu \rightarrow \mu} , \quad (174)$$

$$\vec{x} = [M_\mu^T \hat{d}', \hat{d}] , \quad \vec{y} = (\vec{x})_{\mu \rightarrow \nu} , \quad (175)$$

$$\vec{x}' = [M_\mu \hat{d}, \hat{d}'] , \quad \vec{y}' = (\vec{x}')_{\mu \rightarrow \nu} , \quad (176)$$

$$\Delta X = \hat{d}' \hat{d}^T (\hat{d}'^T M_\nu \hat{d}) - M_\nu \hat{d} \hat{d}^T - \hat{d}' \hat{d}'^T M_\nu + M_\nu , \quad \Delta Y = (\Delta X)_{\nu \rightarrow \mu} . \quad (177)$$

proof:

Just algebra.

QED

Theorem 27 See Fig.10.

$$M_\nu^T \vec{y}' = Y_o \vec{x} , \quad M_\mu \vec{x} = X_o \vec{y}' , \quad (178a)$$

$$M_\mu^T \vec{x}' = X_o \vec{y} , \quad M_\nu \vec{y} = Y_o \vec{x}' . \quad (178b)$$

proof:

Just algebra.

QED

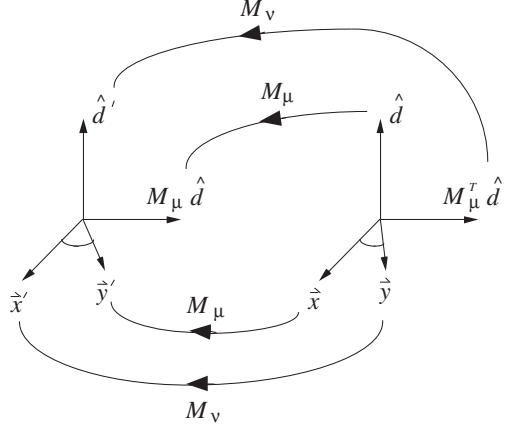


Figure 10: Various vectors and what they are mapped into (up to a scalar factor) by M_μ and M_ν . Since $M_\nu^T M_\mu$ and $M_\mu^T M_\nu$ are both proportional to the identity matrix, one can replace M_μ by M_ν^T and M_ν by M_μ^T in this figure if one also reverses the direction of the mapping arrows.

9 Identities for Circuits with 2 Qubits

This section deals with 2-qubit circuits, whereas Section 10 deals with 3-qubit ones. In this section, with its numerous subsections, we start to reap the benefits of all our preceding hard work. The combination of dressed CNOTs and the LO-RHS invariant proves to be very useful. We find simple-to-check necessary and sufficient conditions for the reduction of a quantum circuit with j CNOTs to fewer CNOTs, where $j = 2, 3$. Plus we show how to express circuits with 1 or 2 controlled-U's as circuits with 2 or fewer CNOTs. Plus we show how to open and close a breach, a procedure that can reduce any 4-CNOT circuit to a 3-CNOT one.

9.1 Reducing 2 DC-NOTs

9.1.1 2 to 2 DC-NOTs (Angle Swapping)

[swap_angles.m, test_swang.m]

In this section we consider a circuit with 2 DC-NOTs acting on 2 qubits, and show that a symmetry in $\mathcal{G}_2^{(2)}$ allows one to swap certain angles without changing the effect of the circuit (up to LO-RHS).

As motivation for the main theorem of this section (the Angle Swapping Theorem), we present the next theorem. The next theorem shows that the target and control qubits of a controlled-U can be exchanged.

Theorem 28 *For any $\theta \in \mathbb{R}$,*

$$\begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} e^{i\theta\sigma_{\hat{b}'}} \text{---} \end{array} = \begin{array}{c} \text{---} e^{i\theta\sigma_{\hat{a}}} \text{---} e^{-i\frac{\theta}{2}\sigma_{\hat{a}}} \text{---} \\ | \\ \text{---} \hat{b}' \text{---} e^{+i\frac{\theta}{2}\sigma_{\hat{b}'}} \text{---} \end{array} . \quad (179)$$

proof:

$$[e^{i\theta\sigma_{\hat{b}'}}(1)]^{n_{\hat{a}}(0)} = e^{i\theta\sigma_{\hat{b}'}}(1) \left(\frac{1-\sigma_{\hat{a}}(0)}{2} \right) \quad (180a)$$

$$= e^{i\theta\sigma_{\hat{a}}(0)} \left(\frac{1-\sigma_{\hat{b}'}(1)}{2} \right) e^{-i\frac{\theta}{2}\sigma_{\hat{a}}(0)} e^{+i\frac{\theta}{2}\sigma_{\hat{b}'}(1)} \quad (180b)$$

$$= [e^{i\theta\sigma_{\hat{a}}}(0)]^{n_{\hat{b}'}(1)} e^{-i\frac{\theta}{2}\sigma_{\hat{a}}(0)} e^{+i\frac{\theta}{2}\sigma_{\hat{b}'}(1)} . \quad (180c)$$

QED

The previous theorem immediately implies the next one, which states that we can “swap a breach” between two qubits.

Theorem 29 *(Swapping a breach) Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{a} \text{---} \parallel \text{---} \hat{a} \text{---} \\ | \quad | \\ \text{---} \hat{p}' \text{---} \text{---} \hat{q}' \text{---} \end{array} , \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{p} \text{---} \text{---} \hat{q} \text{---} \\ | \quad | \\ \text{---} \hat{b}' \text{---} \parallel \text{---} \hat{b}' \text{---} \end{array} . \quad (181)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_{\mathcal{R}} \mathcal{R}$.

proof:

Define θ to be the angle between \hat{p}' and \hat{q}' , and \hat{b} the direction of $\hat{p}' \times \hat{q}'$. Then $\hat{p}' \cdot \hat{q}' = \cos(\theta)$ and $\hat{p}' \times \hat{q}' = \sin(\theta)\hat{b}'$ so $\sigma_{\hat{p}'}\sigma_{\hat{q}'} = e^{i\theta\sigma_{\hat{b}'}}$. Thus,

$$\begin{array}{c} \text{---} \hat{a} \text{---} \parallel \text{---} \hat{a} \text{---} \\ | \quad | \\ \text{---} \hat{p}' \text{---} \text{---} \hat{q}' \text{---} \end{array} = \begin{array}{c} \text{---} \hat{a} \text{---} \\ | \\ \text{---} e^{i\theta\sigma_{\hat{b}'}} \text{---} \end{array} . \quad (182)$$

Given a unit vector \hat{a} and an angle θ , we can always find (non-unique) unit vectors \hat{p} and \hat{q} such that $\text{angle}(\hat{p}, \hat{q}) = \theta$, and $\hat{p} \times \hat{q}$ points along \hat{a} . Then $\hat{p} \cdot \hat{q} = \cos(\theta)$ and $\hat{p} \times \hat{q} = \sin(\theta)\hat{a}$ so $\sigma_{\hat{p}}\sigma_{\hat{q}} = e^{i\theta\sigma_{\hat{a}}}$. It follows that

$$\begin{array}{c} \text{---} e^{i\theta\sigma_{\hat{a}}} \text{---} \\ | \\ \text{---} \hat{b}' \text{---} \end{array} = \begin{array}{c} \text{---} \hat{p} \text{---} \text{---} \hat{q} \text{---} \\ | \quad | \\ \text{---} \hat{b}' \text{---} \parallel \text{---} \hat{b}' \text{---} \end{array} . \quad (183)$$

Now apply Theorem 28 to Eqs.(182) and (183).

QED

Is it possible to swap a foil instead of a breach? Yes it is. In fact, one can swap any angle, as the following theorem shows.

Theorem 30 (*Angle Swapping*) *Let*

$$\mathcal{L} = \begin{array}{cc} \text{---} \hat{b} \text{---} & \text{---} \hat{a} \text{---} \\ | & | \\ \text{---} \hat{b}' \text{---} & \text{---} \hat{a}' \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{cc} \text{---} \hat{b}_f \text{---} & \text{---} \hat{a}_f \text{---} \\ | & | \\ \text{---} \hat{b}'_f \text{---} & \text{---} \hat{a}'_f \text{---} \end{array}. \quad (184)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$ and such that $\text{angle}(\hat{b}, \hat{a}) = \text{angle}(\hat{b}_f, \hat{a}_f)$ and $\text{angle}(\hat{b}', \hat{a}') = \text{angle}(\hat{b}'_f, \hat{a}'_f)$.

proof:

As proven in Section 8.2, $\mathcal{L}^{(2)}$ can be parameterized as follows:

$$\mathcal{L}^{(2)} = c_{\alpha'} c_{\alpha} - (s_{\alpha'} s_{\alpha}) \hat{f}_2' \hat{f}_2^T + i \begin{array}{c|cc} & \hat{f}_1^T & \hat{f}_3^T \\ \hline \hat{f}_3' & s_{\alpha'} c_{\alpha} & 0 \\ \hat{f}_1' & 0 & c_{\alpha'} s_{\alpha} \end{array}, \quad (185)$$

where $\alpha, \alpha' \in \mathbb{R}$ and where $(\hat{f}_j)_{j=1,2,3}$ and $(\hat{f}_j')_{j=1,2,3}$ are two RHON bases such that

$$\hat{b} = \hat{f}_1, \quad \hat{a} = c_{\alpha} \hat{f}_1 - s_{\alpha} \hat{f}_2, \quad (186)$$

and

$$\hat{b}' = \hat{f}_1', \quad \hat{a}' = c_{\alpha'} \hat{f}_1' - s_{\alpha'} \hat{f}_2'. \quad (187)$$

$\mathcal{R}^{(2)}$ can be parameterized in the same way as $\mathcal{L}^{(2)}$, but with the replacements $\alpha \rightarrow \alpha_f$, $\alpha' \rightarrow \alpha'_f$, $\hat{f}_j \rightarrow (\hat{f}_j)_f$, and $\hat{f}_j' \rightarrow (\hat{f}_j')_f$.

Our goal is to construct an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$. Such an \mathcal{R} , if it exists, must satisfy $\hat{\mathcal{L}}^{(2)} = \pm \hat{\mathcal{R}}^{(2)}$. We will use the positive sign. In light of Eq.(74), this gives

$$i^2 \mathcal{L}^{(2)} = i^2 \mathcal{R}^{(2)}. \quad (188)$$

From the symmetrical form of the parameterized expressions for $\mathcal{L}^{(2)}$ and $\mathcal{R}^{(2)}$, it is clear that these two invariants are equal if their principal parameters are related in the following way:

$$\alpha_f = \alpha', \quad \alpha'_f = \alpha, \quad (189)$$

$$\hat{f}_{3f} = \hat{f}_1, \quad \hat{f}_{1f} = \hat{f}_3, \quad \hat{f}_{2f} = -\hat{f}_2, \quad (190)$$

and

$$\hat{f}'_{3f} = \hat{f}'_1, \quad \hat{f}'_{1f} = \hat{f}'_3, \quad \hat{f}'_{2f} = -\hat{f}'_2. \quad (191)$$

These relations between the principal parameters of $\mathcal{L}^{(2)}$ and $\mathcal{R}^{(2)}$ imply that

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{f}_1 \text{---} \text{---} c_\alpha \hat{f}_1 - s_\alpha \hat{f}_2 \text{---} \\ | \\ \text{---} \hat{f}'_1 \text{---} \text{---} c_{\alpha'} \hat{f}'_1 - s_{\alpha'} \hat{f}'_2 \text{---} \end{array} \quad (192a)$$

$$= \begin{array}{c} \text{---} \hat{b} \text{---} \text{---} \hat{a} \text{---} \\ | \quad | \\ \text{---} \hat{b}' \text{---} \text{---} \hat{a}' \text{---} \end{array}, \quad (192b)$$

and

$$\mathcal{R} = \begin{array}{c} \text{---} \hat{f}_3 \text{---} \text{---} c_{\alpha'} \hat{f}_3 + s_{\alpha'} \hat{f}_2 \text{---} \\ | \\ \text{---} \hat{f}'_3 \text{---} \text{---} c_\alpha \hat{f}'_3 + s_\alpha \hat{f}'_2 \text{---} \end{array} \quad (193a)$$

$$= \begin{array}{c} \text{---} \frac{[\hat{a}\hat{b}]}{s_\alpha} \text{---} \text{---} \frac{c_{\alpha'}[\hat{a}\hat{b}] + s_{\alpha'}[\hat{a}\hat{b}\hat{b}]}{s_\alpha} \text{---} \\ | \\ \text{---} \frac{[\hat{a}'\hat{b}']}{s_{\alpha'}} \text{---} \text{---} \frac{c_\alpha[\hat{a}'\hat{b}'] + s_\alpha[\hat{a}'\hat{b}'\hat{b}']}{s_{\alpha'}} \text{---} \end{array}. \quad (193b)$$

(Eq.(193b) is valid only if s_α and $s_{\alpha'}$ are both non-zero, whereas Eq.(193a) is always valid. Theorem 29 corresponds to the case $s_\alpha = 0$.)

We are done proving the theorem, but we will go one step further, and give the value of the local operations $U', U \in SU(2)$ such that

$$\mathcal{L} = \mathcal{R}(U'^\dagger \otimes U^\dagger). \quad (194)$$

When $\hat{f}_1 = \hat{f}'_1 = \hat{x}$ and $\hat{f}_3 = \hat{f}'_3 = \hat{z}$, the right-hand sides of Eqs.(192a) and (193a) appear in Theorem 11. It follows from Theorem 11 and Eq.(40) that

$$U = e^{i\frac{\alpha}{2}\sigma_{\hat{f}_3}} e^{-i\frac{\alpha'}{2}\sigma_{\hat{f}_1}}, \quad U' = (U)_{\alpha \leftrightarrow \alpha', \hat{f} \rightarrow \hat{f}'}. \quad (195)$$

QED

9.1.2 2 to 1 DC-NOTs

In this section, we give necessary and sufficient conditions for a circuit with 2 DC-NOTs acting on 2 qubits to reduce to 1 DC-NOT.



Figure 11: All circuits with 2 DC-NOTs that reduce to 1 DC-NOT.

Theorem 31 *Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{a}_f \text{---} \\ | \\ \text{---} \hat{a}'_f \text{---} \end{array}. \quad (196)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$ if and only if $(\hat{b} \parallel \hat{a} \text{ and } \hat{b}' \perp \hat{a}')$ or $(\hat{b} \perp \hat{a} \text{ and } \hat{b}' \parallel \hat{a}')$. See Fig.11.

proof:

(\Leftarrow)

Suppose $\hat{b} \perp \hat{a}$ and $\hat{b}' \parallel \hat{a}'$ (the other case is analogous). When $\hat{b} \perp \hat{a}$,

$$\sigma_{\hat{b}}(0)^{n_{\hat{a}'(1)}} \sigma_{\hat{a}}(0)^{n_{\hat{a}'(1)}} = [i\sigma_{\hat{b} \times \hat{a}}(0)]^{n_{\hat{a}'(1)}}. \quad (197)$$

The last equation can be expressed diagrammatically as

$$\begin{array}{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \hat{a}' \text{---} \end{array} \begin{array}{c} \perp \\ \parallel \end{array} = \begin{array}{c} \text{---} \hat{b} \times \hat{a} \text{---} \\ | \\ \text{---} \hat{a}' \text{---} \boxed{i^{n_{\hat{a}'}}} \text{---} \end{array}. \quad (198)$$

Thus, when $\hat{b} \perp \hat{a}$ and $\hat{b}' = \hat{a}'$, \mathcal{L} reduces to a single DC-NOT. More generally, $\hat{a}' = \pm \hat{b}'$. Let \mathcal{L}_{new} be a new circuit obtained by replacing in \mathcal{L} : \hat{a}' by its negative if $\hat{a}' = -\hat{b}'$. By virtue of Eq.(25), $\mathcal{L} = \mathcal{L}_{new}(I_2 \otimes U)$, where $U \in U(2)$. If $\mathcal{L}_{new} \sim_R \mathcal{R}_{new}$, then $\mathcal{L} \sim_R \mathcal{R}_{new}$.

(\Rightarrow)

$\mathcal{L} \sim_R \mathcal{R}$ so $\hat{\mathcal{L}}^{(2)} = \pm \hat{\mathcal{R}}^{(2)}$. In light of Eq.(74), this gives

$$i^2 \mathcal{L}^{(2)} = \pm i \mathcal{R}^{(2)}. \quad (199)$$

It follows that

$$\lambda_{2r} + \Lambda_{2r} + i\Lambda_{2i} = \pm i\sigma_{\hat{a}'_f, \hat{a}_f}, \quad (200)$$

where

$$\lambda_{2r} = (\hat{a} \cdot \hat{b})(\hat{a}' \cdot \hat{b}'), \quad (201)$$

$$\Lambda_{2r} = -\sigma_{[\hat{a}'\hat{b}'\hat{b}'], [\hat{a}\hat{b}\hat{b}]} , \quad (202)$$

$$\Lambda_{2i} = \hat{a} \cdot \hat{b} \sigma_{\hat{a}' \times \hat{b}', \hat{b}} + \hat{a}' \cdot \hat{b}' \sigma_{\hat{b}', \hat{a} \times \hat{b}} . \quad (203)$$

$\lambda_{2r} = 0$ so $\hat{a} \cdot \hat{b} = 0$ or $\hat{a}' \cdot \hat{b}' = 0$. Assume the former (the other case is analogous). Then $\hat{a} \perp \hat{b}$. $\Lambda_{2r} = 0$ and $\hat{a} \cdot \hat{b} = 0$ so $[\hat{a}'\hat{b}'\hat{b}'] = 0$, which in turn implies that $\hat{a}' \parallel \hat{b}'$.

QED

9.1.3 2 to 0 DC-NOTs

In this section, we give necessary and sufficient conditions for a circuit with 2 DC-NOTs acting on 2 qubits to reduce to zero DC-NOTs (i.e., to merely local operations).

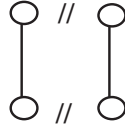


Figure 12: All circuits with 2 DC-NOTs that reduce to 0 DC-NOTs.

Theorem 32 *Suppose*

$$\mathcal{L} = \begin{array}{cc} \text{---} \hat{b} \text{---} & \text{---} \hat{a} \text{---} \\ | & | \\ \text{---} \hat{b}' \text{---} & \text{---} \hat{a}' \text{---} \end{array} . \quad (204)$$

For any \mathcal{L} , $\mathcal{L} \sim_R 1$ if and only if $\hat{a} \parallel \hat{b}$ and $\hat{a}' \parallel \hat{b}'$. See Fig.12.

proof:

(\Leftarrow)

When $\hat{a} = \hat{b}$ and $\hat{a}' = \hat{b}'$, \mathcal{L} equals 1. More generally, $\hat{a} = \pm \hat{b}$ and $\hat{a}' = \pm \hat{b}'$. Let \mathcal{L}_{new} be a new circuit obtained by replacing in \mathcal{L} : (1) \hat{a} by its negative if $\hat{a} = -\hat{b}$, (2) \hat{a}' by its negative if $\hat{a}' = -\hat{b}'$. By virtue of Eq.(25), $\mathcal{L} = \mathcal{L}_{new}(U' \otimes U)$, where $U', U \in U(2)$. If $\mathcal{L}_{new} \sim_R 1$, then $\mathcal{L} \sim_R 1$.

(\Rightarrow)

$\mathcal{L} \sim_R 1$ so $\hat{\mathcal{L}}^{(2)} = \pm 1$. In light of Eq.(74), this gives

$$i^2 \mathcal{L}^{(2)} = \pm 1 . \quad (205)$$

It follows that

$$\lambda_{2r} + \Lambda_{2r} + i\Lambda_{2i} = \pm 1 . \quad (206)$$

Thus $\lambda_{2r} = (\hat{a} \cdot \hat{b})(\hat{a}' \cdot \hat{b}') = \pm 1$, which implies $\hat{a} \parallel \hat{b}$ and $\hat{a}' \parallel \hat{b}'$.

QED

9.2 Reducing 3 DC-NOTs

9.2.1 3 to 2 DC-NOTs

[dr_3to2.m, test_dr_3to2.m]

In this section, we give necessary and sufficient conditions for a circuit with 3 DC-NOTs acting on 2 qubits to reduce to 2 DC-NOTs.

The constraint $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0$ shows up below. The field of Spherical Geometry sheds some light on this constraint. If we connect the points $\hat{a}, \hat{b}, \hat{c}$ by mayor-circle arcs on the unit sphere, then we get what is called a spherical triangle. $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0$ if and only if this spherical triangle has a right angle at vertex \hat{b} . (See Fig.14 for an example of $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$.)

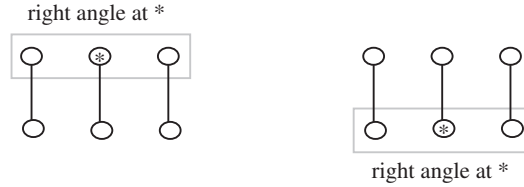


Figure 13: All circuits with 3 DC-NOTs that reduce to 2 DC-NOTs.

Theorem 33 *Suppose*

$$\mathcal{L} = \begin{array}{c} \hat{c} \quad \hat{b} \quad \hat{a} \\ | \\ \hat{c}' \quad \hat{b}' \quad \hat{a}' \end{array}, \quad \mathcal{R} = \begin{array}{c} \hat{b}_f \quad \hat{a}_f \\ | \\ \hat{b}'_f \quad \hat{a}'_f \end{array}. \quad (207)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$ if and only if either $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0$ or $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$. See Fig.13.

proof:

Before we start the proof in earnest, let us restate some pertinent formulas taken from previous sections.

From Section 8.2, we know that

$$\mathcal{R}^{(2)} = \lambda_{2r} + \Lambda_{2r} + i\Lambda_{2i} \quad (208a)$$

$$= c_{\alpha'} c_{\alpha} - (s_{\alpha'} s_{\alpha}) \hat{f}'_2 \hat{f}_2^T + i \begin{array}{c|cc} & \hat{f}_1^T & \hat{f}_3^T \\ \hline \hat{f}'_3 & s_{\alpha'} c_{\alpha} & 0 \\ \hat{f}'_1 & 0 & c_{\alpha'} s_{\alpha} \end{array}. \quad (208b)$$

From Section 8.3, we know that

$$\mathcal{L}^{(2)} = \lambda_{3r} + i\lambda_{3i} + \Lambda_{3r} + i\Lambda_{3i}, \quad (209)$$

where

$$\lambda_{3r} = [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' \quad [\hat{a}\hat{b}\hat{b}] \cdot \hat{c} , \quad (210)$$

$$\lambda_{3i} = -(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})\mathcal{V}' - (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\mathcal{V} , \quad (211)$$

$$\Lambda_{3r} = \begin{cases} -(\hat{a}' \cdot \hat{b}')(\hat{a} \cdot \hat{b})\hat{c}'\hat{c}^T \\ +(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})[\hat{a}'\hat{b}'\hat{c}']\hat{c}^T + (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\hat{c}'[\hat{a}\hat{b}\hat{c}]^T \\ +(\hat{a}' \cdot \hat{b}')\mathcal{V}[\hat{b}'\hat{c}']\hat{c}^T + (\hat{a} \cdot \hat{b})\mathcal{V}'\hat{c}'[\hat{b}\hat{c}]^T \\ -[\hat{a}'\hat{b}'\hat{b}'\hat{c}'\hat{c}'][\hat{a}\hat{b}\hat{b}\hat{c}\hat{c}]^T , \end{cases} \quad (212)$$

and

$$\Lambda_{3i} = \begin{cases} +(\hat{a} \cdot \hat{b})[\hat{a}'\hat{b}'\hat{c}'\hat{c}'][\hat{b}\hat{c}\hat{c}]^T + (\hat{a}' \cdot \hat{b}')[\hat{b}'\hat{c}'\hat{c}'][\hat{a}\hat{b}\hat{c}\hat{c}]^T \\ +[\hat{a}\hat{b}\hat{b}] \cdot \hat{c}[\hat{a}'\hat{b}'\hat{b}'\hat{c}']\hat{c}^T + [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}'\hat{c}'[\hat{a}\hat{b}\hat{b}\hat{c}]^T \end{cases} . \quad (213)$$

Now we begin the proof in earnest.

(\Rightarrow)

$\mathcal{L} \sim_R \mathcal{R}$ so $\hat{\mathcal{L}}^{(2)} = \pm \hat{\mathcal{R}}^{(2)}$. In light of Eq.(74), this gives

$$i^3 \mathcal{L}^{(2)} = \pm i^2 \mathcal{R}^{(2)} . \quad (214)$$

It follows that

$$0 = \lambda_{3r} = [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' \quad [\hat{a}\hat{b}\hat{b}] \cdot \hat{c} . \quad (215)$$

Thus, either $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}'$ or $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c}$.

(\Leftarrow)

Assume $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$. (The other case, $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0$, is analogous).

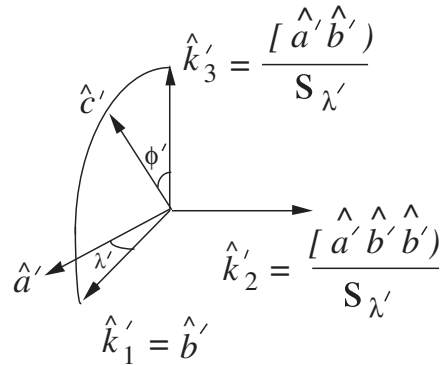


Figure 14: Vectors and angles associated with bit-1 space spanned by \hat{a}' , \hat{b}' , \hat{c}' .

It is convenient at this point to define a RHON basis $(\hat{k}'_j)_{j=1,2,3}$ for the 3d real space spanned by $\hat{a}', \hat{b}', \hat{c}'$. Let $s_{\lambda'} = |[\hat{a}'\hat{b}']|$. If $s_{\lambda'} \neq 0$, let

$$(\hat{k}'_j)_{j=1,2,3} = (\hat{b}', \frac{[\hat{a}'\hat{b}'\hat{b}']}{s_{\lambda'}}, \frac{[\hat{a}'\hat{b}']}{s_{\lambda'}}). \quad (216)$$

If $s_{\lambda'} = 0$, define $(\hat{k}'_j)_{j=1,2,3}$ to be any RHON basis such that $\hat{k}'_1 = \hat{b}'$ and \hat{k}'_2 is perpendicular to $\text{span}(\hat{b}', \hat{c}')$. Let $\phi' = \text{angle}(\hat{c}', \hat{k}'_3)$. Since $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$,

$$\hat{a}' = c_{\lambda'}\hat{k}'_1 - s_{\lambda'}\hat{k}'_2, \quad \hat{b}' = \hat{k}'_1, \quad \hat{c}' = s_{\phi'}\hat{k}'_1 + c_{\phi'}\hat{k}'_3. \quad (217)$$

Eqs.(216) and (217) are illustrated in Fig.14.

Our goal is to construct an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$. Such an \mathcal{R} must satisfy $\hat{\mathcal{L}}^{(2)} = \pm \hat{\mathcal{R}}^{(2)}$. We will use the positive sign. In light of Eq.(74), this gives

$$i^3 \mathcal{L}^{(2)} = i^2 \mathcal{R}^{(2)}. \quad (218)$$

It follows that:

$$\lambda_{2r} = -\lambda_{3i}, \quad (219a)$$

$$0 = \lambda_{3r}, \quad (219b)$$

$$\Lambda_{2r} = -\Lambda_{3i}, \quad (219c)$$

$$\Lambda_{2i} = \Lambda_{3r}. \quad (219d)$$

By evaluating Eq.(219a), we get

$$c_{\alpha'}c_{\alpha} = (\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})\mathcal{V}' + (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\mathcal{V} \quad (220a)$$

$$= (\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})s_{\lambda'}c_{\phi'} + c_{\lambda'}s_{\phi'}\mathcal{V}. \quad (220b)$$

Eq.(219b) is satisfied since $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$ by assumption.

By evaluating Eq.(219c), we get

$$-s_{\alpha'}s_{\alpha}\hat{f}'_2\hat{f}_2^T = \begin{cases} -(\hat{a} \cdot \hat{b})[\hat{a}'\hat{b}'\hat{c}'][\hat{b}\hat{c}\hat{c}]^T \\ -(\hat{a}' \cdot \hat{b}')[\hat{b}'\hat{c}'\hat{c}'][\hat{a}\hat{b}\hat{c}\hat{c}]^T \\ -[\hat{a}\hat{b}\hat{b}] \cdot \hat{c}[\hat{a}'\hat{b}'\hat{b}'\hat{c}']\hat{c}^T \end{cases}. \quad (221)$$

Define \vec{h} by

$$\vec{h} = \begin{cases} +s_{\lambda'}s_{\phi'}(\hat{a} \cdot \hat{b})[\hat{b}\hat{c}\hat{c}]^T \\ -c_{\lambda'}c_{\phi'}[\hat{a}\hat{b}\hat{c}\hat{c}]^T \\ +s_{\lambda'}[\hat{a}\hat{b}\hat{b}] \cdot \hat{c}\hat{c}^T \end{cases}. \quad (222)$$

If $s_{\lambda'} \neq 0$ and $|\vec{h}| \neq 0$, let

$$s_{\alpha'} s_{\alpha} = |\vec{h}|, \quad \hat{f}'_2 = \frac{[\hat{a}'\hat{b}'\hat{c}']}{s_{\lambda'}}, \quad \hat{f}_2 = \frac{\vec{h}}{|\vec{h}|}. \quad (223)$$

If $|\vec{h}| = 0$, set $s_{\alpha'} s_{\alpha} = 0$ and choose any unit vectors for \hat{f}_2 and \hat{f}'_2 . If $|\vec{h}| \neq 0$ but $s_{\lambda'} = 0$, keep Eq.(223) for $s_{\alpha'} s_{\alpha}$ and \hat{f}_2 but use $\hat{f}'_2 = \hat{k}'_2 \times \hat{c}'$.

By evaluating Eq.(219d), we get

$$\Lambda_{2i} = \hat{c}' \vec{v}_1^T + \hat{k}'_2 \vec{v}_2^T, \quad (224)$$

where

$$\vec{v}_1 = -c_{\lambda'}(\hat{a} \cdot \hat{b})\hat{c} + c_{\lambda'} s_{\phi'}[\hat{a}\hat{b}\hat{c}] + s_{\lambda'} c_{\phi'}(\hat{a} \cdot \hat{b})[\hat{b}\hat{c}], \quad (225a)$$

and

$$\vec{v}_2 = s_{\lambda'} s_{\phi'}(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})\hat{c} - c_{\lambda'} c_{\phi'} \mathcal{V}\hat{c} + s_{\lambda'}[\hat{a}\hat{b}\hat{c}\hat{c}]. \quad (225b)$$

At this point, we can follow from step 3 to the end of the Algorithm for Diagonalizing $\mathcal{G}_2^{(2)}$ that was given in Section 8.2. This will yield values for \hat{a}_f , \hat{a}'_f , \hat{b}_f , and \hat{b}'_f .

QED

Compared with the previous Theorem, the next theorem imposes more constraints on \mathcal{L} , and obtains a more constrained \mathcal{R} .

Theorem 34 *Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \\ \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{b}_f \text{---} \hat{a}_f \text{---} \\ | \quad | \\ \text{---} \hat{b}'_f \text{---} \hat{a}'_f \text{---} \end{array}. \quad (226)$$

Let $\lambda' = \text{angle}(\hat{a}', \hat{b}')$ and $\phi' = \text{angle}(\hat{c}', \hat{a}' \times \hat{b}')$. For any \mathcal{L} , if

$$[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0, \quad (227a)$$

and

$$\left[c_{\phi'}(\hat{a} \cdot \hat{b})[\hat{a}\hat{b}] - s_{\lambda'} c_{\lambda'} s_{\phi'} \hat{b} \right] \cdot \hat{c} = 0, \quad (227b)$$

then it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$ and such that $\hat{b}'_f = \hat{c}'$. (Hence, \hat{c}' “persists”, from initial circuit \mathcal{L} to final circuit \mathcal{R} , as the bottom defining vector of the leftmost DC-NOT for both circuits.)

proof:

The (\Leftarrow) part of the proof of the previous theorem still applies.

Using the definitions of \vec{v}_1 and \vec{v}_2 given by Eqs.(225), it is not hard to show that

$$\vec{v}_1^T \vec{v}_2 = 0 \iff \left[c_{\phi'}(\hat{a} \cdot \hat{b})[\hat{a}\hat{b}] - s_{\lambda'} c_{\lambda'} s_{\phi'} \hat{b} \right] \cdot \hat{c} = 0. \quad (228)$$

Since \vec{v}_1 and \vec{v}_2 are orthogonal, the singular values and singular vectors of Λ_{2i} can be obtained simply by inspection of Eq.(224). If $|\hat{v}_1| \neq 0$ and $|\hat{v}_2| \neq 0$, then one can immediately set

$$\hat{f}'_3 = \hat{k}'_2, \quad \hat{f}_1 = \frac{\vec{v}_2}{|\vec{v}_2|}, \quad s_{\alpha'} c_{\alpha} = |\vec{v}_2|, \quad (229)$$

and

$$\hat{f}'_1 = \hat{c}', \quad \hat{f}_3 = \frac{\vec{v}_1}{|\vec{v}_1|}, \quad c_{\alpha'} s_{\alpha} = |\vec{v}_1|. \quad (230)$$

If $|\vec{v}_1| = 0$ but $|\vec{v}_2| \neq 0$, choose $\hat{f}_3 = \hat{f}_1 \times \hat{f}_2$. If $|\vec{v}_1| \neq 0$ but $|\vec{v}_2| = 0$, choose $\hat{f}_1 = \hat{f}_2 \times \hat{f}_3$. If $|\vec{v}_1| = 0$ and $|\vec{v}_2| = 0$, choose \hat{f}_1 and \hat{f}_3 to be any vectors that make $(\hat{f}_j)_{j=1,2,3}$ a RHON basis.

QED

9.2.2 3 to 1 DC-NOTs

In this section, we give necessary and sufficient conditions for a circuit with 3 DC-NOTs acting on 2 qubits to reduce to 1 DC-NOT.

Theorem 35 *Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \\ \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{a}_f \text{---} \\ | \\ \text{---} \hat{a}'_f \text{---} \end{array}. \quad (231)$$

Let $\mathcal{V} = \hat{a} \times \hat{b} \cdot \hat{c}$, and $\mathcal{V}' = \hat{a}' \times \hat{b}' \cdot \hat{c}'$. For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$ if and only if one or more of the following are true: (See Fig.15)

$$T_{1a} : (\hat{b} \parallel \hat{a}) \text{ and } (\hat{b}' \parallel \hat{a}')$$

$$T_{1b} : (\hat{c} \parallel \hat{b}) \text{ and } (\hat{c}' \parallel \hat{b}')$$

$$T_{2a} : (\hat{c}' \parallel \hat{b}' \parallel \hat{a}') \text{ and } \mathcal{V} = 0$$

$$T_{2b} : (\hat{c} \parallel \hat{b} \parallel \hat{a}) \text{ and } \mathcal{V}' = 0$$

$$T_{3a} : \hat{a} \perp \text{span}(\hat{b}, \hat{c}) \text{ and } \hat{a}' \perp \text{span}(\hat{b}', \hat{c}')$$

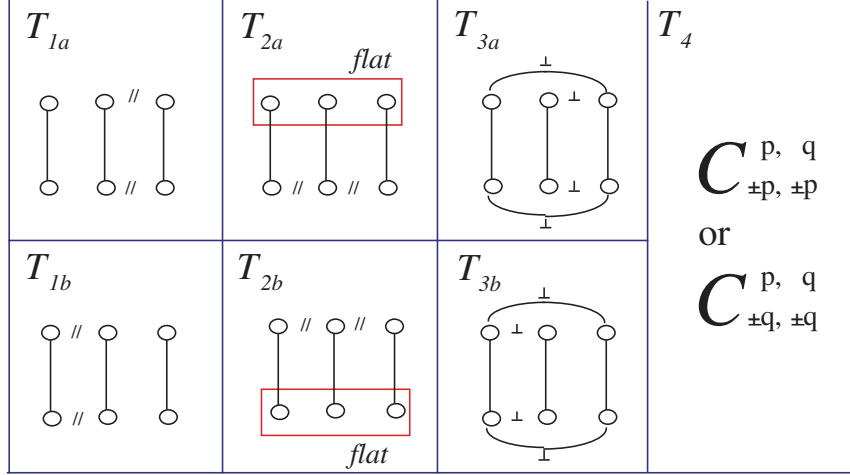


Figure 15: All circuits with 3 DC-NOTs that reduce to 1 DC-NOTs. The 8 circuits $\mathcal{C}_{\pm p, \pm p}^{p, q}$ and $\mathcal{C}_{\pm q, \pm q}^{p, q}$ are defined by Eq.(237).

$$T_{3b} : \hat{c} \perp \text{span}(\hat{a}, \hat{b}) \text{ and } \hat{c}' \perp \text{span}(\hat{a}', \hat{b}')$$

$$T_4 : \begin{cases} [\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0 \text{ and } [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0 \\ \frac{|\hat{a} \times \hat{b}|}{|\hat{a} \cdot \hat{b}|} = \frac{|\hat{a}' \times \hat{b}'|}{|\hat{a}' \cdot \hat{b}'|} \text{ and } \frac{|\hat{b} \times \hat{c}|}{|\hat{b} \cdot \hat{c}|} = \frac{|\hat{b}' \times \hat{c}'|}{|\hat{b}' \cdot \hat{c}'|} \\ \text{sign} \left(\frac{\mathcal{V}}{(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})} \right) = - \text{sign} \left(\frac{\mathcal{V}'}{(\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')} \right) \end{cases} . \quad (232)$$

proof:

(\Leftarrow)

Consider a circuit of type T_{1b} (T_{1a} case is analogous). When $\hat{c} = \hat{b}$ and $\hat{c}' = \hat{b}'$, it is obvious that a T_{1b} circuit reduces to a single DC-NOT. More generally, $\hat{c} = \pm \hat{b}$ and $\hat{c}' = \pm \hat{b}'$. Let \mathcal{L}_{new} be a new circuit obtained by replacing in \mathcal{L} : (1) \hat{c} by its negative if $\hat{c} = -\hat{b}$, (2) \hat{c}' by its negative if $\hat{c}' = -\hat{b}'$. By virtue of Eq.(25), $\mathcal{L} = (U' \otimes U)\mathcal{L}_{new}$, where $U', U \in U(2)$. If $\mathcal{L}_{new} \sim_R \mathcal{R}_{new}$, then $\mathcal{L} \sim_R (U' \otimes U)\mathcal{R}_{new}(U'^{\dagger} \otimes U^{\dagger})$.

Now consider a circuit of type T_{2a} (T_{2b} case is analogous). Note that when $\mathcal{V} = 0$,

$$\sigma_{\hat{c}}\sigma_{\hat{b}}\sigma_{\hat{a}} = \sigma_{(\hat{a} \cdot \hat{b})\hat{c} - [\hat{a}\hat{b}\hat{c}]} = \sigma_{\hat{a}_f} , \quad (233)$$

so

$$\begin{array}{c} \hat{c} \quad \hat{b} \quad \hat{a} \\ \circ \quad \circ \quad \circ \\ \text{---} \quad \text{---} \quad \text{---} \\ | \quad | \quad | \\ \hat{a}' \quad \hat{a}' \quad \hat{a}' \\ \circ \quad \circ \quad \circ \end{array} = \begin{array}{c} \boxed{\sigma_{\hat{c}}\sigma_{\hat{b}}\sigma_{\hat{a}}} \\ \text{---} \\ \hat{a}' \\ \circ \end{array} = \begin{array}{c} \hat{a}_f \\ \circ \\ \text{---} \\ | \\ \hat{a}' \\ \circ \end{array} . \quad (234)$$

Circuits of type T_{3a} (T_{3b} case is analogous) reduce to a single DC-NOT by virtue of Theorem 10.

$$|\tan \lambda| = |\tan \lambda'| \quad \text{and} \quad |\tan \phi| = |\tan \phi'|, \quad (235)$$
$$\text{sign}\left(\frac{\tan \lambda}{\tan \phi}\right) = -\text{sign}\left(\frac{\tan \lambda'}{\tan \phi'}\right). \quad (236)$$
$$\mathcal{C}_{(-1)^{m_r}, (-1)^{n_r}}^{p,q} = \begin{array}{c} \text{---} \hat{p}_{zx}^\phi \text{---} \hat{x} \text{---} \hat{q}_{xy}^\lambda \text{---} \\ | \quad \quad \quad | \\ \text{---} (-1)^{m_r} r_{zx}^\phi \text{---} \hat{x} \text{---} (-1)^{n_r} r_{xy}^\lambda \text{---} \end{array}, \quad (237)$$
$$\begin{array}{c|c|c|c|c}
\phi' = \downarrow, \lambda' = \Rightarrow & \lambda & \pi - \lambda & \pi + \lambda & -\lambda \\
\hline
\phi & \times & \mathcal{C}_{p,-p}^{p,q} & \times & \mathcal{C}_{p,p}^{p,q} \\
\hline
\pi - \phi & \mathcal{C}_{-q,q}^{p,q} & \times & \mathcal{C}_{-q,-q}^{p,q} & \times \\
\hline
\pi + \phi & \times & \mathcal{C}_{-p,-p}^{p,q} & \times & \mathcal{C}_{-p,p}^{p,q} \\
\hline
-\phi & \mathcal{C}_{q,q}^{p,q} & \times & \mathcal{C}_{q,-q}^{p,q} & \times
\end{array} . \quad (238)$$

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For $\mathcal{C}_{q,q}^{p,q}$ (ditto, for $\mathcal{C}_{p,p}^{p,q}$), there exists an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$ by virtue of Eq.(56) (ditto, Eq.(66)). The other 6 circuits of table Eq.(238) can be handled as follows. Let \mathcal{L}_{new} be a new circuit obtained by replacing in \mathcal{L} : (1) λ' by $\lambda' - \pi$ if $\lambda' = \pi \pm \lambda \pmod{2\pi}$, (2) ϕ' by $\phi' - \pi$ if $\phi' = \pi \pm \phi \pmod{2\pi}$. By virtue of Eq.(25), $\mathcal{L} = (U' \otimes U)\mathcal{L}_{new}(V' \otimes V)$ where $U', U, V', V \in U(2)$, and where \mathcal{L}_{new} is of type $\mathcal{C}_{q,q}^{p,q}$ or $\mathcal{C}_{p,p}^{p,q}$. If $\mathcal{L}_{new} \sim_R \mathcal{R}_{new}$, then $\mathcal{L} \sim_R (U' \otimes U)\mathcal{R}_{new}(U'^{\dagger} \otimes U^{\dagger})$.
 (\Rightarrow)

$\mathcal{L} \sim_R \mathcal{R}$ so $\hat{\mathcal{L}}^{(2)} = \pm \hat{\mathcal{R}}^{(2)}$. In light of Eq.(74), this gives

$$i^3 \mathcal{L}^{(2)} = \pm i \mathcal{R}^{(2)} . \quad (239)$$

It follows that

$$\lambda_{3r} + i\lambda_{3i} + \Lambda_{3r} + i\Lambda_{3i} = \pm \sigma_{\hat{a}'_f, \hat{a}_f} , \quad (240)$$

where

$$\lambda_{3r} = [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' \quad [\hat{a}\hat{b}\hat{b}] \cdot \hat{c} , \quad (241)$$

$$\lambda_{3i} = -(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})\mathcal{V}' - (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\mathcal{V} , \quad (242)$$

$$\Lambda_{3r} = \begin{cases} -(\hat{a}' \cdot \hat{b}')(\hat{a} \cdot \hat{b})\hat{c}'\hat{c}^T \\ +(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})[\hat{a}'\hat{b}'\hat{c}']\hat{c}^T + (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\hat{c}'[\hat{a}\hat{b}\hat{c}]^T \\ +(\hat{a}' \cdot \hat{b}')\mathcal{V}[\hat{b}'\hat{c}']\hat{c}^T + (\hat{a} \cdot \hat{b})\mathcal{V}'\hat{c}'[\hat{b}\hat{c}]^T \\ -[\hat{a}'\hat{b}'\hat{b}'\hat{c}'\hat{c}'][\hat{a}\hat{b}\hat{b}\hat{c}\hat{c}]^T , \end{cases} \quad (243)$$

and

$$\Lambda_{3i} = \begin{cases} +(\hat{a} \cdot \hat{b})[\hat{a}'\hat{b}'\hat{c}'\hat{c}'][\hat{b}\hat{c}\hat{c}]^T + (\hat{a}' \cdot \hat{b}')[\hat{b}'\hat{c}'\hat{c}'][\hat{a}\hat{b}\hat{c}\hat{c}]^T \\ +[\hat{a}\hat{b}\hat{b}] \cdot \hat{c}[\hat{a}'\hat{b}'\hat{b}'\hat{c}']\hat{c}^T + [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}'\hat{c}'[\hat{a}\hat{b}\hat{b}\hat{c}]^T \end{cases} . \quad (244)$$

First assume that there are no breaches in \mathcal{L} (i.e., $\hat{a} \nparallel \hat{b}$, $\hat{b} \nparallel \hat{c}$, $\hat{a}' \nparallel \hat{b}'$, $\hat{b}' \nparallel \hat{c}'$).

Note that

$$[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0 \quad \text{and} \quad [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0 . \quad (245)$$

This is why. From $\lambda_{3r} = 0$, we must have either $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0$ or $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$. But if one of these holds, then the other one follows. Indeed, assume $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0$. Since also $[\hat{a}\hat{b}] \neq 0$, it follows that $[\hat{a}\hat{b}\hat{b}\hat{c}] \neq 0$. From $\Lambda_{3i} = 0$, $\hat{c}^T \Lambda_{3i} = [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}'[\hat{a}\hat{b}\hat{b}\hat{c}]^T = 0$ so $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$. By an analogous argument, assuming $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$ leads to $[\hat{a}\hat{b}\hat{b}] \cdot \hat{c} = 0$.

Next note that

$$\hat{a} \cdot \hat{b} = \hat{a}' \cdot \hat{b}' = 0 \Rightarrow \hat{a} \cdot \hat{c} = \hat{a}' \cdot \hat{c}' = 0 , \quad (246a)$$

and

$$\hat{c} \cdot \hat{b} = \hat{c}' \cdot \hat{b}' = 0 \Rightarrow \hat{c} \cdot \hat{a} = \hat{c}' \cdot \hat{a}' = 0 . \quad (246b)$$

Eqs.(246) become obvious if one uses the BAC minus CAB identity to expand Eqs.(245).

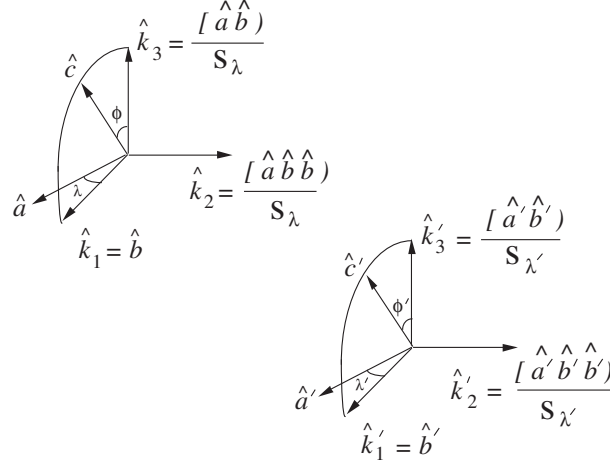


Figure 16: Vectors and angles associated with bit-0 space spanned by $\hat{a}, \hat{b}, \hat{c}$. Vectors and angles associated with bit-1 space spanned by $\hat{a}', \hat{b}', \hat{c}'$.

It is convenient at this point to define a RHON basis $(\hat{k}'_j)_{j=1,2,3}$ for the 3d real space spanned by $\hat{a}', \hat{b}', \hat{c}'$. Let $s_{\lambda'} = |[\hat{a}'\hat{b}']|$. If $s_{\lambda'} \neq 0$, let

$$(\hat{k}'_j)_{j=1,2,3} = (\hat{b}', \frac{[\hat{a}'\hat{b}'\hat{b}']}{s_{\lambda'}}, \frac{[\hat{a}'\hat{b}']}{s_{\lambda'}}) . \quad (247)$$

If $s_{\lambda'} = 0$, let $(\hat{k}'_j)_{j=1,2,3}$ be any RHON basis such that $\hat{k}'_1 = \hat{b}'$ and \hat{k}'_2 is perpendicular to $span(\hat{b}', \hat{c}')$. Let $\phi' = angle(\hat{c}', \hat{k}'_3)$. Since $[\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}' = 0$,

$$\hat{a}' = c_{\lambda'} \hat{k}'_1 - s_{\lambda'} \hat{k}'_2, \quad \hat{b}' = \hat{k}'_1, \quad \hat{c}' = s_{\phi'} \hat{k}'_1 + c_{\phi'} \hat{k}'_3 . \quad (248)$$

Eqs.(247) and (248) are illustrated in Fig.16.

Use the previous paragraph with all the primes removed to define angles λ, ϕ and a RHON basis $(\hat{k}_j)_{j=1,2,3}$ for the 3d real space spanned by $\hat{a}, \hat{b}, \hat{c}$.

When expressed in terms of λ, λ', ϕ and ϕ' , the constraint $\lambda_{3i} = 0$ reduces to

$$-[s_{\lambda'} c_{\lambda} c_{\phi'} s_{\phi} + c_{\lambda'} s_{\lambda} s_{\phi'} c_{\phi}] = 0 . \quad (249)$$

Likewise, the constraint $\Lambda_{3i} = 0$ reduces to

$$-[s_{\lambda'} c_{\lambda} s_{\phi'} c_{\phi} + c_{\lambda'} s_{\lambda} c_{\phi'} s_{\phi}][\hat{k}'_2 \hat{c}'](\hat{k}_2 \hat{c})^T = 0 . \quad (250)$$

Eqs.(249) and (250) imply the following system of 2 equations:

$$\begin{bmatrix} c_{\phi'} s_{\phi} & s_{\phi'} c_{\phi} \\ s_{\phi'} c_{\phi} & c_{\phi'} s_{\phi} \end{bmatrix} \begin{bmatrix} s_{\lambda'} c_{\lambda} \\ c_{\lambda'} s_{\lambda} \end{bmatrix} = 0 . \quad (251)$$

This system of equations can also be rewritten in the form:

$$\begin{bmatrix} c_{\lambda'} s_{\lambda} & s_{\lambda'} c_{\lambda} \\ s_{\lambda'} c_{\lambda} & c_{\lambda'} s_{\lambda} \end{bmatrix} \begin{bmatrix} s_{\phi'} c_{\phi} \\ c_{\phi'} s_{\phi} \end{bmatrix} = 0 . \quad (252)$$

For Eq.(251), either (i)the solution is the zero vector, or (ii)the determinant of the coefficient matrix vanishes. (i)If the solution is zero, then $s_{\lambda'} c_{\lambda} = c_{\lambda'} s_{\lambda} = 0$. Since we are assuming no breaches, $s_{\lambda'} \neq 0$ and $s_{\lambda} \neq 0$, so we must have $c_{\lambda} = c_{\lambda'} = 0$. By virtue of Eq.(246a), this means that the circuit must be of type T_{3a} . (ii) If the determinant is zero, then

$$|\tan \phi| = |\tan \phi'| . \quad (253)$$

We will pursue this possibility later on.

Likewise, for Eq.(252), either (i)the solution is the zero vector, or (ii)the determinant of the coefficient matrix vanishes. (i)If the solution is zero, then $s_{\phi'} c_{\phi} = c_{\phi'} s_{\phi} = 0$. Since we are assuming no breaches, $c_{\phi} \neq 0$ and $c_{\phi'} \neq 0$, so we must have $s_{\phi} = s_{\phi'} = 0$. By virtue of Eq.(246b), this means that the circuit must be of type T_{3b} . (ii) If the determinant is zero, then

$$|\tan \lambda| = |\tan \lambda'| . \quad (254)$$

We will pursue this possibility later on.

Suppose we assume that the circuit \mathcal{L} is not of type T_3 . Then, we have shown that it must satisfy Eqs.(253) and (254). But these two equations are the second line of Eq.(232). To prove that the circuit must be of type T_4 , it remains for us to prove that the third line of Eq.(232) also holds. This third line clearly follows from $\lambda_{3i} = 0$, where λ_{3i} is given by Eq.(242).

Next , assume that there is at least one breach in \mathcal{L} . Without loss of generality, assume there is a breach between \hat{a} and \hat{b} (i.e., $\hat{a} \parallel \hat{b}$).

$\hat{a} \parallel \hat{b}$ implies that $\mathcal{V} = 0$.

The constraint $\lambda_{3i} = 0$ reduces to

$$(\hat{b} \cdot \hat{c})\mathcal{V}' = 0 , \quad (255)$$

which implies that either $\hat{b} \cdot \hat{c} = 0$ or $\mathcal{V}' = 0$. The constraint $\Lambda_{3i} = 0$ reduces to

$$[\hat{a}' \hat{b}' \hat{c}' \hat{c}'](\hat{b} \hat{c} \hat{c})^T = 0 , \quad (256)$$

which implies that either (i) $\hat{b} \parallel \hat{c}$ or (ii) $\hat{a}' \parallel \hat{b}'$ or (iii) $[\hat{a}'\hat{b}'] \parallel \hat{c}'$. (i) If $\hat{b} \parallel \hat{c}$, then, by Eq.(255), $\mathcal{V}' = 0$. ($\hat{a} \parallel \hat{b} \parallel \hat{c}$) and $\mathcal{V}' = 0$ so \mathcal{L} is of type T_{2b} . (ii) If $\hat{a}' \parallel \hat{b}'$, then, since also $\hat{a} \parallel \hat{b}$, \mathcal{L} is of type T_{1a} . (iii) Suppose $[\hat{a}'\hat{b}'] \parallel \hat{c}'$. Assume that $\hat{a}' \not\parallel \hat{b}'$ as the case when these two vectors are parallel has already been considered. It follows that the conditions T_{3b} are satisfied. This is why. $[\hat{a}'\hat{b}'] \parallel \hat{c}'$ and $\hat{a}' \not\parallel \hat{b}'$ imply that $\mathcal{V}' \neq 0$, and, therefore, by virtue of Eq.(255), $\hat{c} \perp \hat{b}$. Now $\hat{c} \perp \hat{b}$ and $\hat{a} \parallel \hat{b}$ imply that $\hat{c} \perp \hat{a}$. Thus, $\hat{c} \perp \text{span}(\hat{b}, \hat{a})$. Also, $[\hat{a}'\hat{b}'] \parallel \hat{c}'$ implies that $\hat{c}' \perp \text{span}(\hat{b}', \hat{a}')$.

QED

9.2.3 3 to 0 DC-NOTs

In this section, we give necessary and sufficient conditions for a circuit with 3 DC-NOTs acting on 2 qubits to reduce to zero DC-NOTs (i.e., to merely local operations).

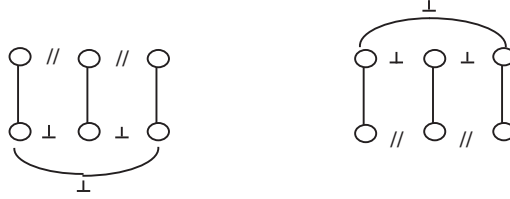


Figure 17: All circuits with 3 DC-NOTs that reduce to 0 DC-NOTs.

Theorem 36 *Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \\ \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \end{array} . \quad (257)$$

For any \mathcal{L} , $\mathcal{L} \sim_R 1$ if and only if one of the following is true (see Fig.17)

T_a : $(\hat{c}', \hat{b}', \hat{a}')$ are mutually orthogonal, and $(\hat{c} \parallel \hat{b} \parallel \hat{a})$

T_b : $(\hat{c}, \hat{b}, \hat{a})$ are mutually orthogonal, and $(\hat{c}' \parallel \hat{b}' \parallel \hat{a}')$

proof:

(\Leftarrow)

Consider a circuit of type T_b (T_a case is analogous). Note that when $(\hat{c}, \hat{b}, \hat{a})$ are mutually orthogonal,

$$\sigma_{\hat{c}} \sigma_{\hat{b}} \sigma_{\hat{a}} = i \hat{c} \cdot [\hat{b} \hat{a}] = \pm i . \quad (258)$$

Hence,

$$\begin{array}{c} \textcircled{\hat{c}} \\ \text{---} \end{array} \begin{array}{c} \textcircled{\hat{b}} \\ \text{---} \end{array} \begin{array}{c} \textcircled{\hat{a}} \\ \text{---} \end{array} = \begin{array}{c} \boxed{\sigma_{\hat{c}} \sigma_{\hat{b}} \sigma_{\hat{a}}} \\ \text{---} \end{array} \begin{array}{c} \textcircled{\hat{a}'} \\ \text{---} \end{array} = \begin{array}{c} \boxed{(\pm i)^{n_{\hat{a}'}}} \\ \text{---} \end{array} . \quad (259)$$

Thus, when $\hat{a}' = \hat{b}' = \hat{c}'$, a T_b circuit reduces to zero DC-NOTs. More generally, $\hat{a}' = \pm \hat{b}'$ and $\hat{c}' = \pm \hat{b}'$. Let \mathcal{L}_{new} be a new circuit obtained by replacing in \mathcal{L} : (1) \hat{a}' by its negative if $\hat{a}' = -\hat{b}'$, (2) \hat{c}' by its negative if $\hat{c}' = -\hat{b}'$. By virtue of Eq.(25), $\mathcal{L} = (I_2 \otimes U) \mathcal{L}_{new} (I_2 \otimes V)$ where $U, V \in U(2)$. If $\mathcal{L}_{new} \sim_R 1$, then $\mathcal{L} \sim_R 1$.

(\Rightarrow)

$\mathcal{L} \sim_R 1$ so $\hat{\mathcal{L}}^{(2)} = \pm 1$. In light of Eq.(74), this gives

$$i^3 \mathcal{L}^{(2)} = \pm 1 . \quad (260)$$

It follows that

$$\lambda_{3r} + i\lambda_{3i} + \Lambda_{3r} + i\Lambda_{3i} = \pm i , \quad (261)$$

where

$$\lambda_{3r} = [\hat{a}' \hat{b}' \hat{c}'] \cdot \hat{c}' \quad [\hat{a} \hat{b} \hat{c}] \cdot \hat{c} , \quad (262)$$

$$\lambda_{3i} = -(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})\mathcal{V}' - (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\mathcal{V} , \quad (263)$$

$$\Lambda_{3r} = \begin{cases} -(\hat{a}' \cdot \hat{b}')(\hat{a} \cdot \hat{b})\hat{c}'\hat{c}^T \\ +(\hat{a} \cdot \hat{b})(\hat{b} \cdot \hat{c})[\hat{a}'\hat{b}'\hat{c}']\hat{c}^T + (\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\hat{c}'[\hat{a}\hat{b}\hat{c}]^T \\ +(\hat{a}' \cdot \hat{b}')\mathcal{V}[\hat{b}'\hat{c}']\hat{c}^T + (\hat{a} \cdot \hat{b})\mathcal{V}'\hat{c}'[\hat{b}\hat{c}]^T \\ -[\hat{a}'\hat{b}'\hat{b}'\hat{c}'\hat{c}'][\hat{a}\hat{b}\hat{b}\hat{c}\hat{c}]^T , \end{cases} \quad (264)$$

and

$$\Lambda_{3i} = \begin{cases} +(\hat{a} \cdot \hat{b})[\hat{a}'\hat{b}'\hat{c}'\hat{c}'][\hat{b}\hat{c}\hat{c}]^T + (\hat{a}' \cdot \hat{b}')[\hat{b}'\hat{c}'\hat{c}'][\hat{a}\hat{b}\hat{c}\hat{c}]^T \\ +[\hat{a}\hat{b}\hat{b}] \cdot \hat{c}[\hat{a}'\hat{b}'\hat{b}'\hat{c}']\hat{c}^T + [\hat{a}'\hat{b}'\hat{b}'] \cdot \hat{c}'\hat{c}'[\hat{a}\hat{b}\hat{b}\hat{c}]^T . \end{cases} \quad (265)$$

$\hat{c}'^T \Lambda_{3r} \hat{c} = 0$ so $\hat{a}' \cdot \hat{b}' = 0$ or $\hat{a} \cdot \hat{b} = 0$. Both can't be true at once or else we would have $\lambda_{3i} = 0$, which is false. Assume henceforth that $\hat{a}' \cdot \hat{b}' \neq 0$ and $\hat{a} \cdot \hat{b} = 0$ (the case $\hat{a}' \cdot \hat{b}' = 0$ and $\hat{a} \cdot \hat{b} \neq 0$ is analogous). When $\hat{a} \cdot \hat{b} = 0$, $|\lambda_{3i}| = 1$ reduces to $|(\hat{a}' \cdot \hat{b}')(\hat{b}' \cdot \hat{c}')\mathcal{V}| = 1$, which immediately implies that $(\hat{c}' \parallel \hat{b}' \parallel \hat{a}')$, and $(\hat{c}, \hat{b}, \hat{a})$ are mutually orthogonal. Thus, circuit \mathcal{L} must be of type T_b .

QED

9.3 Reducing Controlled- U 's

9.3.1 One Controlled- U

In this section, we show that any controlled- U can be expressed with just two CNOTs. This result was first proven by Barenco et al. in Ref.[9]. Their method of proof is long and opaque compared with the ultra simple proof given below. This attests to the benefits of using dressed CNOTs.

Theorem 37 *Let $\theta \in \mathbb{R}$. Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \boxed{e^{i\theta\sigma_{\hat{w}}}} \text{---} \\ | \\ \text{---} \bullet \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{cc} \text{---} \hat{b} \text{---} & \text{---} \hat{a} \text{---} \\ | & | \\ \text{---} \hat{z} \text{---} & \text{---} \hat{z} \text{---} \end{array}. \quad (266)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} = \mathcal{R}$.

proof:

Given a unit vector \hat{w} and an angle θ , we can always find (non-unique) unit vectors \hat{b} and \hat{a} such that $\text{angle}(\hat{b}, \hat{a}) = \theta$, and $\hat{b} \times \hat{a}$ points along \hat{w} . Then $\hat{b} \cdot \hat{a} = \cos(\theta)$ and $\hat{b} \times \hat{a} = \sin(\theta)\hat{w}$ so $\sigma_{\hat{b}}\sigma_{\hat{a}} = e^{i\theta\sigma_{\hat{w}}}$.

$$[e^{i\theta\sigma_{\hat{w}}(0)}]^{n(1)} = [\sigma_{\hat{b}}(0)\sigma_{\hat{a}}(0)]^{n(1)} = \sigma_{\hat{b}}(0)^{n(1)}\sigma_{\hat{a}}(0)^{n(1)}. \quad (267)$$

QED

9.3.2 Two Controlled- U 's (The Deflation Identity)

[deflate_dcnots.m, test_deflate_dcnots.m]

In this section, we show that a product of two controlled- U s can be expressed with just two CNOTs. This “Deflation Identity” was first proven in Ref.[10]. Unlike the proof of Ref.[10], the one below uses dressed CNOTs.

Theorem 38 *Let $A \in SU(2)$ and $\theta_L, \theta_R \in \mathbb{R}$. Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \boxed{e^{i\theta_L\sigma_{\hat{w}_L}}} \text{---} \boxed{e^{i\theta_R\sigma_{\hat{w}_R}}} \text{---} \\ | \qquad \qquad | \\ \text{---} \bullet \text{---} \boxed{A} \text{---} \bullet \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{cc} \text{---} \hat{b}_f \text{---} & \text{---} \hat{a}_f \text{---} \\ | & | \\ \text{---} \hat{b}'_f \text{---} & \text{---} \hat{a}'_f \text{---} \end{array}. \quad (268)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$.

proof:

Given a unit vector \hat{w}_L and an angle θ_L , we can always find (non-unique) unit vectors \hat{d} and \hat{c} such that $\text{angle}(\hat{d}, \hat{c}) = \theta_L$, and $\hat{d} \times \hat{c}$ points along \hat{w}_L . Then $\hat{d} \cdot \hat{c} = \cos(\theta_L)$ and $\hat{d} \times \hat{c} = \sin(\theta_L)\hat{w}_L$ so $\sigma_{\hat{d}}\sigma_{\hat{c}} = e^{i\theta_L\sigma_{\hat{w}_L}}$. Likewise, given a unit vector

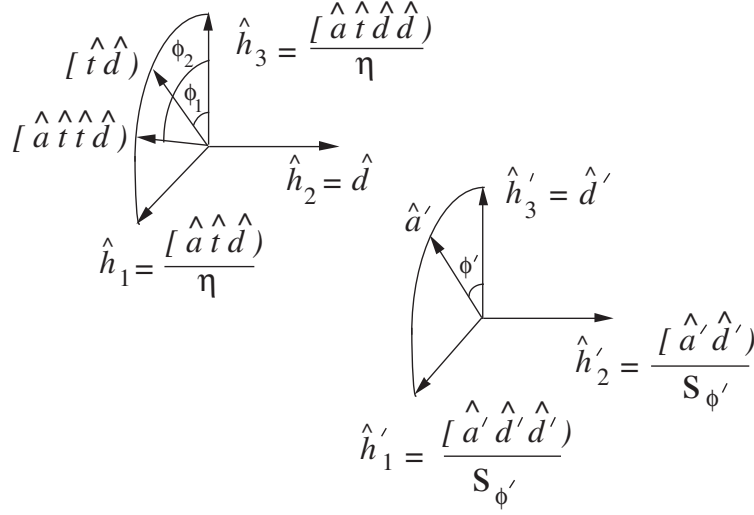


Figure 18: Variables used in Theorem 38.

\hat{w}_L and an angle θ_L , we can always find (non-unique) unit vectors \hat{b} and \hat{a} such that $\sigma_{\hat{b}}\sigma_{\hat{a}} = e^{i\theta_R\sigma_{\hat{w}_R}}$. We are free to rotate the vectors \hat{d} and \hat{c} (ditto, \hat{b} and \hat{a}) within the plane they initially span, as long as we don't change the angle between them. In particular, we can choose both \hat{c} and \hat{b} to lie along the line of intersection between the planes $\text{span}(\hat{d}, \hat{c})$ and $\text{span}(\hat{b}, \hat{a})$. In other words, we can always choose $\hat{c} = \hat{b}$. Call \hat{t} their common value. It is now clear that, without loss of generality, we can replace \mathcal{L} by

$$\mathcal{L} = \begin{array}{ccccccc} & \hat{d} & \hat{t} & \parallel & \hat{t} & \hat{a} & \\ \text{---} & | & | & & | & | & \\ & \hat{d}' & \hat{d}' & \parallel & \hat{a}' & \hat{a}' & \\ & | & | & & | & | & \end{array} . \quad (269)$$

Our goal is to construct an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$. Such an \mathcal{R} , if it exists, must satisfy $\hat{\mathcal{L}}^{(2)} = \pm \hat{\mathcal{R}}^{(2)}$. We will use the positive sign. In light of Eq.(74), this gives

$$i^4 \mathcal{L}^{(2)} = i^2 \mathcal{R}^{(2)} . \quad (270)$$

Using the same calculational techniques that were used in Section 8, one finds

$$\mathcal{L}^{(2)} = \begin{cases} (\hat{a} \cdot \hat{t})(\hat{t} \cdot \hat{d}) - (\hat{a}' \cdot \hat{d}')[\hat{a}\hat{t}\hat{t}] \cdot \hat{d} \\ i \left[(\hat{a} \cdot \hat{t})\hat{d}'[\hat{t}\hat{d}]^T - (\hat{a}' \cdot \hat{d}')\hat{d}'[\hat{a}\hat{t}\hat{t}\hat{d}]^T + [\hat{a}'\hat{d}'\hat{d}'][\hat{a}\hat{t}\hat{d}\hat{d}]^T \right] \\ + [\hat{a}\hat{t}] \cdot \hat{d}[\hat{a}'\hat{d}']\hat{d}^T \end{cases} . \quad (271)$$

From Section 8.2, we know that $\mathcal{R}^{(2)}$ can be expressed as

$$\mathcal{R}^{(2)} = \lambda_{2r} + \Lambda_{2r} + i\Lambda_{2i} \quad (272a)$$

$$= c_{\alpha'} c_{\alpha} - (s_{\alpha'} s_{\alpha}) \hat{f}_2' \hat{f}_2^T + i \begin{array}{c|cc} & \hat{f}_1^T & \hat{f}_3^T \\ \hline \hat{f}_3' & s_{\alpha'} c_{\alpha} & 0 \\ \hat{f}_1' & 0 & c_{\alpha'} s_{\alpha} \end{array}. \quad (272b)$$

We must have

$$\lambda_{2r} = c_{\alpha'} c_{\alpha} = -(\hat{a} \cdot \hat{t})(\hat{t} \cdot \hat{d}) + (\hat{a}' \cdot \hat{d}')[\hat{a}\hat{t}\hat{t}] \cdot \hat{d}, \quad (273)$$

and

$$\Lambda_{2r} = -s_{\alpha'} s_{\alpha} \hat{f}_2' \hat{f}_2^T = -[\hat{a}\hat{t}] \cdot \hat{d} [\hat{a}'\hat{d}'] \hat{d}^T. \quad (274)$$

Define

$$s_{\phi'} = |[\hat{a}'\hat{d}']|, \quad \eta = |[\hat{a}\hat{t}\hat{d}]|. \quad (275)$$

If $s_{\phi'} \neq 0$, Eq.(274) is satisfied by

$$s_{\alpha'} s_{\alpha} = [\hat{a}\hat{t}] \cdot \hat{d} s_{\phi'}, \quad \hat{f}_2' = \frac{[\hat{a}'\hat{d}']}{s_{\phi'}}, \quad \hat{f}_2 = \hat{d}. \quad (276)$$

If $s_{\phi'} = 0$, choose $s_{\alpha} s_{\alpha'}$ and \hat{f}_2 the same way, but choose \hat{f}_2' to be any vector perpendicular to \hat{d}' .

If $s_{\phi'} \neq 0$ and $\eta \neq 0$, define the following two RHON bases (illustrated in Fig.18):

$$(\hat{h}'_j)_{j=1,2,3} = \left(\frac{[\hat{a}'\hat{d}'\hat{d}']}{s_{\phi'}}, \frac{[\hat{a}'\hat{d}']}{s_{\phi'}}, \hat{d}' \right), \quad (277)$$

and

$$(\hat{h}_j)_{j=1,2,3} = \left(\frac{[\hat{a}\hat{t}\hat{d}]}{\eta}, \hat{d}, \frac{[\hat{a}\hat{t}\hat{d}\hat{d}]}{\eta} \right). \quad (278)$$

If $s_{\phi'} = 0$, pick $(\hat{h}'_j)_{j=1,2,3}$ to be any RHON basis such that $\hat{h}'_3 = \hat{d}'$. If $\eta = 0$, pick $(\hat{h}_j)_{j=1,2,3}$ to be any RHON basis such that $\hat{h}_2 = \hat{d}$. Define the following two angles (illustrated in Fig.18):

$$\phi_2 = \text{angle}([\hat{a}\hat{t}\hat{d}], \hat{h}_3), \quad \phi_1 = \text{angle}([\hat{t}\hat{d}], \hat{h}_3). \quad (279)$$

We must have

$$\Lambda_{2i} = -(\hat{a} \cdot \hat{t})\hat{d}'[\hat{t}\hat{d}]^T + (\hat{a}' \cdot \hat{d}')\hat{d}'[\hat{a}\hat{t}\hat{t}\hat{d}]^T - [\hat{a}'\hat{d}'\hat{d}'][\hat{a}\hat{t}\hat{d}\hat{d}]^T \quad (280a)$$

$$= \begin{array}{c|cc} & \hat{h}_1^T & \hat{h}_3^T \\ \hline \hat{h}_3' & -\hat{a} \cdot \hat{t}s_{\phi_1} + c_{\phi'}s_{\phi_2} & -\hat{a} \cdot \hat{t}c_{\phi_1} + c_{\phi'}c_{\phi_2} \\ \hat{h}_1' & 0 & -s_{\phi'}\eta \end{array} . \quad (280b)$$

At this point, we can follow from step 4 to the end of the Algorithm for Diagonalizing $\mathcal{G}_2^{(2)}$ that was given in Section 8.2. This will yield values for \hat{a}_f , \hat{a}'_f , \hat{b}_f , and \hat{b}'_f .

QED

9.4 Opening and Closing a Breach

[breach.m, test_breach.m]

*Once more unto the breach, dear friends, once more; Or close the wall up
with our English dead!* (from “King Henry V” by W. Shakespeare)

In this section, we show how to “open and close a breach” in 2-qubit circuits. This is a procedure whereby one can reduce any 2-qubit circuit with 4 CNOTs into a circuit with 3 CNOTs. Applying this procedure repeatedly, one can reduce any 2-qubit circuit with more than 3 CNOTs into a circuit with only 3 CNOTs. The fact that all 2-qubit circuits can be expressed with 3 (or fewer) CNOTs was first proven in Ref.[6]. Unlike the proof below, their proof was based on Cartan’s KAK decomposition[7].

Theorem 39 (*Opening a Breach*) Suppose

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{p}_L \text{---} \hat{q}_L \text{---} \hat{q}_R \text{---} \hat{p}_R \text{---} \\ | \\ \text{---} \hat{p}'_L \text{---} \hat{q}'_L \text{---} \hat{q}'_R \text{---} \hat{p}'_R \text{---} \end{array} , \quad (281)$$

$$\mathcal{R} = \begin{array}{c} \text{---} \hat{p}_{Lf} \text{---} \hat{q}_{Lf} \text{---} \hat{q}_{Rf} \text{---} \hat{p}_{Rf} \text{---} \\ | \\ \text{---} \hat{p}'_{Lf} \text{---} \hat{t}' \text{---} \hat{t}' \text{---} \hat{p}'_{Rf} \text{---} \end{array} . \quad (282)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$.

proof:

We begin by inserting a “unit wedge” into \mathcal{L} :

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{p}_L \text{---} \hat{q}_L \text{---} \hat{t} \text{---} \hat{t} \text{---} \hat{q}_R \text{---} \hat{p}_R \text{---} \\ | \\ \text{---} \hat{p}'_L \text{---} \hat{q}'_L \text{---} \hat{t}' \text{---} \hat{t}' \text{---} \hat{q}'_R \text{---} \hat{p}'_R \text{---} \end{array} . \quad (283)$$

In Eq.(283), \hat{t} and \hat{t}' are auxiliary parameters whose values are still to be defined.

Consider separately each half of the circuit in Eq.(283). Our goal is to re-express each half as follows:

$$\begin{array}{c} \hat{t} \\ \circ \\ \text{---} \end{array} \begin{array}{c} \hat{q}_R \\ \circ \\ \text{---} \end{array} \begin{array}{c} \hat{p}_R \\ \circ \\ \text{---} \end{array} = \begin{array}{c} \hat{q}_{Rf} \\ \circ \\ \text{---} \end{array} \begin{array}{c} \hat{p}_{Rf} \\ \circ \\ \text{---} \end{array} \begin{array}{c} U_{Rf} \\ \square \\ \text{---} \end{array} , \quad (284)$$

and

$$\begin{array}{c} \hat{p}_L \\ \circ \\ \text{---} \end{array} \begin{array}{c} \hat{q}_L \\ \circ \\ \text{---} \end{array} \begin{array}{c} \hat{t} \\ \circ \\ \text{---} \end{array} = \begin{array}{c} U_{Lf} \\ \square \\ \text{---} \end{array} \begin{array}{c} \hat{p}_{Lf} \\ \circ \\ \text{---} \end{array} \begin{array}{c} \hat{q}_{Lf} \\ \circ \\ \text{---} \end{array} . \quad (285)$$

From Theorem 34, we know that Eq.(284) will be achieved if we constrain our auxiliary parameters by:

$$[\hat{p}'_R \hat{q}'_R \hat{q}'_R] \cdot \hat{t}' = 0 , \quad (286a)$$

and

$$[c_{\phi'_R} (\hat{p}_R \cdot \hat{q}_R) \hat{p}_R \times \hat{q}_R - s_{\lambda'_R} c_{\lambda'_R} s_{\phi'_R} \hat{q}_R] \cdot \hat{t} = 0 . \quad (286b)$$

Likewise, Eq.(285) will be achieved if we constrain our auxiliary parameters by the same pair of equations as Eqs.(286), but with R subscripts replaced by L subscripts. These 4 constraint equations can be used to solve for the 4 degrees of freedom contained in the auxiliary parameters \hat{t} and \hat{t}' .

QED

By a “unit wedge” we mean a circuit element which equals one. An analogous concept is a “partition of unity”. If it equals one, why use it? Because it depends on new, auxiliary parameters, and, by merging the unit wedge with its surroundings, we get a new expression which contains the auxiliary parameters, but is functionally independent of them. We can then choose convenient values for the auxiliary parameters. The net result is that we can transform the original circuit to a new one that performs exactly as the old one but appears different.

Note that in Eq.(283) we used a unit wedge consisting of a single DC-NOT times itself. There was no a priori obvious reason why this unit wedge would lead us to a proof of the theorem. We could have chosen a unit wedge that provided more auxiliary parameters. For instance, we could have chosen a product of 3 DC-NOTs (times the inverse of the product). After all, 1 DC-NOT can express only a limited subset of all possible 2-qubit transformations whereas 3 DC-NOTs can be used to express any of them. For proving the above theorem, using a unit wedge with only 1 DC-NOT turned out to be sufficient. But one can envisage this theorem proving technique being used elsewhere with more complicated unit wedges.

Suppose one starts with a circuit which, like \mathcal{L} in Eq.(281), possesses 4 DC-NOTs. By the last theorem, one can “open a breach” in it; that is, transform it into a circuit which, like \mathcal{R} in Eq.(282), possesses two adjacent oval nodes both carrying a \hat{t}' . Then one can combine the two adjacent DC-NOTs with a \hat{t}' node and obtain a controlled-U. Finally, one can use the Deflation Identity of Sec.9.3.2 to express the just created controlled-U and an adjacent DC-NOT as a circuit with two CNOTs. The net effect of this procedure is to reduce any 2-qubit circuit with 4 CNOTs into one with 3 CNOTs.

10 Identities for Circuits with 3 Qubits

10.1 Pass-Through Identities

In the following 3 subsections, we consider the following 3 “identities” (one subsection per identity):

$$\begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array} \sim_R \begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array}, \quad (287a)$$

$$\begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array} \sim_R \begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array}, \quad (287b)$$

$$\begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array} \sim_R \begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array}. \quad (287c)$$

Note that in all 3 identities, the initial and final circuits both have the same number of DC-NOTs, acting on the same 3 qubits. In all 3 cases, we pass a DC-NOT (the mobile one) acting on qubits 0 and 1 through another DC-NOT (the static one) acting on qubits 0 and 2. Thus, the mobile and static DC-NOTs both act on qubit 0, but the second qubit on which they act differs. We will refer to Eq.(287a), Eq.(287b), and Eq.(287c) as the Pass-Through Identities 1,2, and 3, respectively. In the initial circuit of Pass-Through Identity n , the mobile DC-NOT is part of a group of n adjacent DC-NOTs acting on qubits 0 and 1.

The Pass-Through Identities Eqs.(287) do not, per se, change the number of DC-NOTs. However, in some situations, they can be used to reduce the number of DC-NOTs. For example,

$$\begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array} \sim_R \begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array} \quad (288a)$$

$$\sim_R \begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ | \\ \text{---} \bigcirc \text{---} \end{array}. \quad (288b)$$

In Eq.(288a), there are initially 3 adjacent DC-NOTs on the LHS of the static DC-NOT. Using Pass-Through Identity 1, we produce 4 adjacent DC-NOTs on the LHS of the static DC-NOT. As shown in Section 9.4, these 4 adjacent DC-NOTs can always be reduced to 3 DC-NOTs.

10.1.1 Pass-Through Identity 1

Theorem 40 *Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \\ \text{---} \hat{a}' \text{---} \\ | \\ \text{---} \hat{b}'' \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{a}_f \text{---} \hat{b}_f \text{---} \\ | \quad | \\ \text{---} \hat{a}'_f \text{---} \\ | \\ \text{---} \hat{b}''_f \text{---} \end{array}. \quad (289)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$ if and only if $\hat{a} \parallel \hat{b}$.

proof:

(\Leftarrow) Let $\hat{a}'_f = \hat{a}'$ and $\hat{b}''_f = \hat{b}''$. Clearly, if $\hat{a} = \hat{b}$, then $\mathcal{L} = \mathcal{R}$. More generally, $\hat{a} = \pm \hat{b}$. Let \mathcal{L}_{new} be a new circuit obtained by replacing in \mathcal{L} : \hat{a} by its negative if $\hat{a} = -\hat{b}$. By virtue of Eq.(25), $\mathcal{L} = \mathcal{L}_{new}(I_2 \otimes U \otimes I_2)$ where $U \in U(2)$. If $\mathcal{L}_{new} \sim_R \mathcal{R}_{new}$, then $\mathcal{L} \sim_R \mathcal{R}_{new}$.

(\Rightarrow)

Using the same calculational techniques that were used in Section 8, one finds

$$\mathcal{L}^{(2)} = \hat{a} \cdot \hat{b} \sigma_{\hat{b}'', \hat{a}', 1} + i \sigma_{1, \hat{a}', [\hat{a}\hat{b}]}, \quad (290)$$

and

$$\mathcal{R}^{(2)} = \hat{b}_f \cdot \hat{a}_f \sigma_{\hat{b}''_f, \hat{a}'_f, 1} + i \sigma_{\hat{b}''_f, 1, [\hat{a}_f \hat{b}_f]}. \quad (291)$$

$\mathcal{L} \sim_R \mathcal{R}$ implies that $\mathcal{L}^{(2)}$ is proportional to $\mathcal{R}^{(2)}$. Therefore, $\sigma_{1, \hat{a}', [\hat{a}\hat{b}]}$ must vanish. Hence, $[\hat{a}\hat{b}] = 0$, which implies $\hat{a} \parallel \hat{b}$.

QED

10.1.2 Pass-Through Identity 2

Theorem 41 *Suppose*

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{e} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \\ \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \\ | \\ \text{---} \hat{e}'' \text{---} \end{array}, \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{b}_f \text{---} \hat{e}_f \text{---} \hat{a}_f \text{---} \\ | \quad | \quad | \\ \text{---} \hat{b}'_f \text{---} \hat{a}'_f \text{---} \\ | \\ \text{---} \hat{e}''_f \text{---} \end{array}. \quad (292)$$

For any \mathcal{L} , if there exists \hat{t}' such that

$$\begin{array}{c} \hat{e} \quad \hat{b} \quad \hat{a} \\ | \\ \hat{t}' \quad \hat{b}' \quad \hat{a}' \end{array} \sim_R \begin{array}{c} \hat{a}_f \\ | \\ \hat{a}'_f \end{array}, \quad (293)$$

then it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$.

proof:

One has

$$\mathcal{L} = \begin{array}{c} \hat{e} \quad \hat{e} \quad \hat{e} \quad \hat{b} \quad \hat{a} \\ | \\ \hat{t}' \quad \hat{t}' \quad \hat{t}' \quad \hat{b}' \quad \hat{a}' \\ | \\ \hat{e}'' \end{array} \quad (294a)$$

$$= \begin{array}{c} \hat{e} \quad \hat{e} \quad \hat{e} \quad \hat{b} \quad \hat{a} \\ | \\ \hat{t}' \quad \hat{t}' \quad \hat{t}' \quad \hat{b}' \quad \hat{a}' \\ | \\ \hat{e}'' \end{array} \quad (294b)$$

$$= \begin{array}{c} \hat{e} \quad \hat{e} \quad \hat{a}_f \\ | \\ \hat{t}' \quad \hat{t}' \quad \hat{a}'_f \\ | \\ \hat{e}'' \end{array}. \quad (294c)$$

In (a), we introduced a unit wedge. To go from (a) to (b), we passed half of that unit wedge across the “static” DC-NOT. Finally, to go from (b) to (c), we used Eq.(293).

QED

Note that Section 9.2.2 gives necessary and sufficient conditions for a 2-qubit circuit with 3 DC-NOTs to reduce to an equivalent circuit with 1 DC-NOT. Using those necessary and sufficient conditions, it is easy to check in any particular instance whether there exists a \hat{t}' such that Eq.(293) is satisfied.

10.1.3 Pass-Through Identity 3

[pass3.m, test_pass3.m]

Theorem 42 *Suppose*

$$\mathcal{L} = \begin{array}{c} \hat{e} \quad \hat{c} \quad \hat{b} \quad \hat{a} \\ | \\ \hat{c}' \quad \hat{b}' \quad \hat{a}' \\ | \\ \hat{e}'' \end{array}, \quad \mathcal{R} = \begin{array}{c} \hat{c}_f \quad \hat{e}_f \quad \hat{b}_f \quad \hat{a}_f \\ | \\ \hat{c}'_f \quad \hat{b}'_f \quad \hat{a}'_f \\ | \\ \hat{e}''_f \end{array}. \quad (295)$$

For any \mathcal{L} , it is possible to find an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$.

proof:

$$\mathcal{L} = \begin{array}{c} \text{---} \hat{e} \text{---} \hat{e} \text{---} \hat{e} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \quad | \quad | \\ \text{---} \hat{t}' \text{---} \hat{t}' \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \\ | \\ \text{---} \hat{e}'' \text{---} \end{array} \quad (296a)$$

$$= \begin{array}{c} \text{---} \hat{e} \text{---} \hat{e} \text{---} \hat{e} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \quad | \quad | \\ \text{---} \hat{t}' \text{---} \hat{t}' \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \\ | \\ \text{---} \hat{e}'' \text{---} \end{array} \quad (296b)$$

$$= \begin{array}{c} \text{---} \hat{e} \text{---} \hat{e} \text{---} \hat{b}_f \text{---} \hat{a}_f \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \hat{t}' \text{---} \hat{t}' \text{---} \hat{b}'_f \text{---} \hat{a}'_f \text{---} \\ | \\ \text{---} \hat{e}'' \text{---} \end{array} . \quad (296c)$$

In (a), we introduced a unit wedge. To go from (a) to (b), we passed half of that unit wedge across the “static” DC-NOT. Finally, to go from (b) to (c), we used Theorem 43.

QED

The next theorem is used in the proof of Theorem 42.

Theorem 43 *Suppose*

$$\mathcal{L}(\hat{d}') = \begin{array}{c} \text{---} \hat{d} \text{---} \hat{c} \text{---} \hat{b} \text{---} \hat{a} \text{---} \\ | \quad | \quad | \quad | \\ \text{---} \hat{d}' \text{---} \hat{c}' \text{---} \hat{b}' \text{---} \hat{a}' \text{---} \end{array} , \quad \mathcal{R} = \begin{array}{c} \text{---} \hat{b}_f \text{---} \hat{a}_f \text{---} \\ | \quad | \\ \text{---} \hat{b}'_f \text{---} \hat{a}'_f \text{---} \end{array} . \quad (297)$$

For any $\mathcal{L}(\cdot)$, there exists a \hat{d}' and an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$.

proof:

Our goal is to find a \hat{d}' and to construct an \mathcal{R} such that $\mathcal{L} \sim_R \mathcal{R}$. Such an \mathcal{R} must satisfy $\hat{\mathcal{L}}^{(2)} = \pm \hat{\mathcal{R}}^{(2)}$. We will use the positive sign. In light of Eq.(74), the following must be true:

$$i^4 \mathcal{L}^{(2)} = i^2 \mathcal{R}^{(2)} . \quad (298)$$

From Section 8.4, we know that

$$\mathcal{L}^{(2)} = \lambda_{4r} + i\lambda_{4i} + \Lambda_{4r} + i\Lambda_{4i} , \quad (299)$$

where

$$\lambda_{4r} = -\hat{d}'^T M_\nu \hat{d} , \quad (300)$$

$$\lambda_{4i} = -\hat{d}'^T M_\mu \hat{d} , \quad (301)$$

$$\Lambda_{4r} = X_o \hat{d}' \hat{d}^T + \vec{x}' \hat{d}^T + \hat{d}' \vec{x}^T + \Delta X , \quad (302)$$

$$\Lambda_{4i} = Y_o \hat{d}' \hat{d}^T - \vec{y}' \hat{d}^T - \hat{d}' \vec{y}^T + \Delta Y . \quad (303)$$

The precise definitions of (X_o, Y_o) , $(\vec{x}, \vec{x}', \vec{y}, \vec{y}')$, $(\Delta X, \Delta Y)$, and (M_μ, M_ν) in terms of (\hat{a}, \hat{a}') , (\hat{b}, \hat{b}') , (\hat{c}, \hat{c}') , and (\hat{d}, \hat{d}') are given in Section 8.4.

From Section 8.2, we know that

$$\mathcal{R}^{(2)} = \lambda_{2r} + \Lambda_{2r} + i\Lambda_{2i} \quad (304a)$$

$$= c_{\alpha'} c_\alpha - (s_{\alpha'} s_\alpha) \hat{f}_2' \hat{f}_2^T + i \frac{\hat{f}_3'}{\hat{f}_1'} \left| \begin{array}{cc} \hat{f}_1^T & \hat{f}_3^T \\ s_{\alpha'} c_\alpha & 0 \\ 0 & c_{\alpha'} s_\alpha \end{array} \right. . \quad (304b)$$

We must have

$$\lambda_{2r} = -\lambda_{4r} , \quad (305a)$$

$$0 = \lambda_{4i} , \quad (305b)$$

$$\Lambda_{2r} = -\Lambda_{4r} , \quad (305c)$$

and

$$\Lambda_{2i} = -\Lambda_{4i} . \quad (305d)$$

To begin, we will assume that $X_o \neq 0$. Later on, before ending the proof, we will remove this assumption.

By evaluating Eq.(305a), we get

$$c_{\alpha'} c_\alpha = \hat{d}'^T M_\nu \hat{d} . \quad (306)$$

By evaluating Eq.(305b), we get

$$0 = \hat{d}'^T M_\mu \hat{d} . \quad (307)$$

Let \hat{d}' be any unit vector that satisfies this equation.

By evaluating Eq.(305c), we get

$$-s_{\alpha'} s_{\alpha} \hat{f}'_2 \hat{f}_2^T = -(X_o \hat{d}' \hat{d}^T + \vec{x}' \vec{x}^T + \hat{d}' \vec{x}^T + \Delta X) . \quad (308)$$

For Eq.(308) to be true, the RHS of that equation must factor into the product of a column vector times a row vector:

$$-s_{\alpha'} s_{\alpha} \hat{f}'_2 \hat{f}_2^T = -X_o \left(\hat{d}' + \frac{\vec{x}'}{X_o} \right) \left(\hat{d} + \frac{\vec{x}}{X_o} \right)^T . \quad (309)$$

Let

$$s_{\alpha'} s_{\alpha} = X_o \eta'_2 \eta_2 , \quad \hat{f}'_2 = \frac{\hat{d}' + \frac{\vec{x}'}{X_o}}{\eta'_2} , \quad \hat{f}_2 = \frac{\hat{d} + \frac{\vec{x}}{X_o}}{\eta_2} , \quad (310)$$

where

$$\eta'_2 = \left| \hat{d}' + \frac{\vec{x}'}{X_o} \right| = \sqrt{1 + \frac{(\vec{x}')^2}{(X_o)^2}} , \quad \eta_2 = (\eta'_2)_{\text{omit primes}} . \quad (311)$$

Note that since Eqs.(308) and (309) are both true, the following must be true:

$$\frac{\vec{x}' \vec{x}^T}{X_o} = \Delta X . \quad (312)$$

Eq.(312) can also be proven by expressing it in terms of (\hat{a}, \hat{a}') , (\hat{b}, \hat{b}') , (\hat{c}, \hat{c}') , and (\hat{d}, \hat{d}') .

By evaluating Eq.(305d), we get

$$\Lambda_{2i} = -(Y_o \hat{d}' \hat{d}^T - \vec{y}' \vec{d}^T - \hat{d}' \vec{y}^T + \Delta Y) . \quad (313)$$

At this point, we can follow from step 3 to the end of the Algorithm for Diagonalizing $\mathcal{G}_2^{(2)}$ that was given in Section 8.2. This will yield values for \hat{a}_f , \hat{a}'_f , \hat{b}_f , and \hat{b}'_f .

Now assume $X_o = 0$. By Eq.(312), either $\vec{x}' = 0$ or $\vec{x} = 0$. When $\vec{x}' = 0$ and $\vec{x} \neq 0$ (the case $\vec{x}' \neq 0$ and $\vec{x} = 0$ is analogous), Eq.(309) becomes

$$-s_{\alpha'} s_{\alpha} \hat{f}'_2 \hat{f}_2^T = - \left(\hat{d}' + \frac{\vec{x}'}{X_o} \right) \vec{x}^T , \quad (314)$$

where $\frac{\vec{x}'}{X_o}$ is defined as the obvious limit. Thus, we can set

$$s_{\alpha'} s_{\alpha} = \eta'_2 |\vec{x}| , \quad \hat{f}'_2 = \frac{\hat{d}' + \frac{\vec{x}'}{X_o}}{\eta'_2} , \quad \hat{f}_2 = \frac{\vec{x}}{|\vec{x}|} . \quad (315)$$

If $\vec{x}' = \vec{x} = 0$, then Eq.(309) becomes $-s_{\alpha'} s_{\alpha} \hat{f}'_2 \hat{f}_2^T = 0$, so we can set $s_{\alpha'} s_{\alpha} = 0$ and define \hat{f}_2 and \hat{f}'_2 to be arbitrary unit vectors.

Additional observations:

Note that $\hat{f}_2'^T \Lambda_{2i} = 0$ implies

$$\vec{x}' \cdot \vec{y}' = X_o Y_o , \quad (316a)$$

and

$$\Delta Y^T \vec{x}' = X_o \vec{y}' . \quad (316b)$$

Likewise, note that $\Lambda_{2i} \hat{f}_2 = 0$ implies

$$\vec{x} \cdot \vec{y} = X_o Y_o , \quad (317a)$$

and

$$\Delta Y \vec{x} = X_o \vec{y}' . \quad (317b)$$

Eqs.(316) and (317) can also be proven by expressing them in terms of (\hat{a}, \hat{a}') , (\hat{b}, \hat{b}') , (\hat{c}, \hat{c}') , and (\hat{d}, \hat{d}') .

If $|\vec{x}|$ and $|\vec{x}'|$ are both non-zero, it is possible to introduce 2 RHON bases $(\hat{h}'_j)_{j=1,2,3}$ and $(\hat{h}_j)_{j=1,2,3}$, defined as follows. Define \hat{h}'_2 and \hat{h}_2 by

$$\hat{h}'_2 = \hat{f}'_2 , \quad \hat{h}_2 = \hat{f}_2 . \quad (318)$$

Define \hat{h}'_3 and \hat{h}_3 by

$$\hat{h}'_3 = \frac{\hat{d}' - \frac{\vec{x}' X_o}{(\vec{x}')^2}}{\eta'_3} , \quad \hat{h}_3 = (\hat{h}'_3)_{\text{omit primes}} , \quad (319)$$

where

$$\eta'_3 = \left| \hat{d}' - \frac{\vec{x}' X_o}{(\vec{x}')^2} \right| = \sqrt{1 + \frac{(X_o)^2}{(\vec{x}')^2}} = \frac{X_o}{|\vec{x}'|} \eta_2 , \quad \eta_3 = (\eta'_3)_{\text{omit primes}} . \quad (320)$$

Define \hat{h}'_1 and \hat{h}_1 by

$$\hat{h}'_1 = \frac{[\vec{x}' \hat{d}'] \text{sign}(X_o)}{\eta'_1} , \quad \hat{h}_1 = (\hat{h}'_1)_{\text{omit primes}} , \quad (321)$$

where

$$\eta'_1 = |[\vec{x}' \hat{d}']| = |\vec{x}'| , \quad \eta_1 = (\eta'_1)_{\text{omit primes}} . \quad (322)$$

After some algebra, one can show that Eq.(313) becomes

$$\Lambda_{2i} = \frac{\frac{\hat{h}_1^T}{|\vec{x}|} \quad \hat{h}_3^T \eta_3}{\frac{\hat{h}'_3 \eta'_3}{|\vec{x}'|} \begin{vmatrix} \vec{y}^T[\vec{x}\hat{d}] \text{sign}(X_o) & -Y_o \\ -[\vec{x}'\hat{d}']^T \Delta Y[\vec{x}\hat{d}] & \vec{y}'^T[\vec{x}'\hat{d}'] \text{sign}(X_o) \end{vmatrix}}. \quad (323)$$

The entries of the previous table can be expressed solely in terms of (\hat{d}, \hat{d}') and (M_μ, M_ν) . After some algebra, one finds that

$$\vec{y}^T[\vec{x}\hat{d}] = (M_\nu^T \hat{d}') \cdot [M_\mu^T \hat{d}', \hat{d}], \quad (324)$$

$$\vec{y}'^T[\vec{x}'\hat{d}'] = (M_\nu \hat{d}) \cdot [M_\mu \hat{d}, \hat{d}'], \quad (325)$$

and

$$[\vec{x}'\hat{d}']^T \Delta Y[\vec{x}\hat{d}] = \hat{d}^T M_\mu^T M_\mu M_\mu^T \hat{d}'. \quad (326)$$

QED

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